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**A KINETIC MODEL OF SODIUM-WATER REACTION
APPLIED TO DYNAMIC SIMULATION OF LEAK DETECTION
IN THE CORE COMPONENTS TEST LOOP**

by

D. Saphier

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D. Saphier*

July 1976

*On leave from the Israel Atomic Energy Commission Soreq Nuclear
Research Centre

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A KINETIC MODEL OF SODIUM-WATER REACTION APPLIED TO DYNAMIC SIMULATION OF LEAK DETECTION IN THE CORE COMPONENTS TEST LOOP

by

D. Saphier

ABSTRACT

A detailed model for the CCTL steam-generator leak-detection simulation was developed to predict the hydrogen- and oxygen-detector response during a series of experiments to be performed at ANL. The detailed kinetic equations for the sodium-water interaction are given, as well as the assumptions made in assessing the various reactivity rates and hydrogen-gas migration in the sodium toward a free surface in contact with the cover gas. A dynamic model was developed describing concentration changes as a result of primary and secondary sodium reactions, sodium flow through the system piping, mixing processes in various plenum elements, cold-trap operation, cover-gas pressure changes, and water leaks. A computer program CCTL-DYSP has been written in which the dynamic model was simulated to obtain the concentration of the different reaction products as functions of time for any segment of the CCTL system. A generalized approach was used in the modeling and programming procedures, so that only the input data have to be changed in order to analyze different experiments and different system configurations. With minor changes, the computer program can be adapted to simulate leak detection in the CRBR. Some representative results are included in the report, and qualitatively they are in agreement with similar results published elsewhere. Some experimental results also became available recently, and they are in good agreement with the simulated concentrations.

I. INTRODUCTION

The hazard to LMFBR steam generators from small water leaks has long been recognized and has been the subject of several theoretical and experimental studies.¹⁻¹² Large water leaks in a superheater or evaporator will lead to a spontaneous violent reaction and to subsequent partial or complete destruction of the steam generator. Small leaks, if permitted to continue during a period sufficiently long, will produce corrosive agents that cause destructive

wastage of the steam-generator tubing and finally result in "secondary" large leaks with extensive damage. It is, therefore, of utmost importance to detect the small leaks and their location so that the plant can be shut down before significant damage occurs.

Accordingly, an experimental leak-detection program¹ is underway in the Argonne Core Components Test Loop (CCTL) to evaluate methods for small-leak detection. The purpose of this experimental program is to evaluate the most efficient means for detecting water-to-sodium leaks in the range of 10^{-7} - 10^{-3} lb/sec and to gather enough experimental data on the leak-detection methods so that they can be applied to the Clinch River Breeder Reactor (CRBR). A series of experiments, as described in Ref. 1, to simulate water leaks in the CRBR heat exchangers will be performed. These experiments will be carried out under different flow rates, sodium temperatures, leak rates, and leak positions.

The purpose of the present study is to develop a mathematical model for the CCTL leak-detection experiment, and to set up a simulation program capable of solving the model equations in order that the leak-detector response can be predicted with reasonable accuracy. The modeling and the program are set up in a general way so that the CCTL experiment is a particular case. The computer program is modular and with minor changes can be applied to the simulation of other systems having water leaks into a sodium loop.

Several investigators^{1,6,8,10,12} have formulated general relationships between the size of the water leak and the quantity of hydrogen to be found in sodium after steady-state conditions are established. However, these relationships are usually system-dependent. In contrast, the mathematical model for the CCTL leak-detection experiment was developed from basic principles of conservation and the kinetic equations of the chemical reactions. Where certain basic parameters, such as reaction rates and hydrogen-gas disengagement rates, were not well known, reasonable assumptions were introduced. These assumptions can later be checked and improved by appropriate experiments. With this approach, the simulation program is rendered system-independent and can easily be expanded to simulate leak detection in the CRBRP or other sodium systems.

II. THE CCTL LEAK-DETECTION EXPERIMENTAL SETUP

The Core Components Test Loop (CCTL) as well as the leak-detection experimental program are described in Ref. 1. Briefly, the CCTL is a large isothermal sodium loop, as is shown schematically in Fig. 1. The sodium is circulated through the main loop by a mechanical pump having a capacity of 800 gpm. The major component is a large sodium tank within which a simulated module of an CRBRP steam generator is placed. The water and steam pipes are simulated by solid stainless steel rods of the same diameter as the actual pipe. Water leaks are simulated by steam injections made directly into the module.

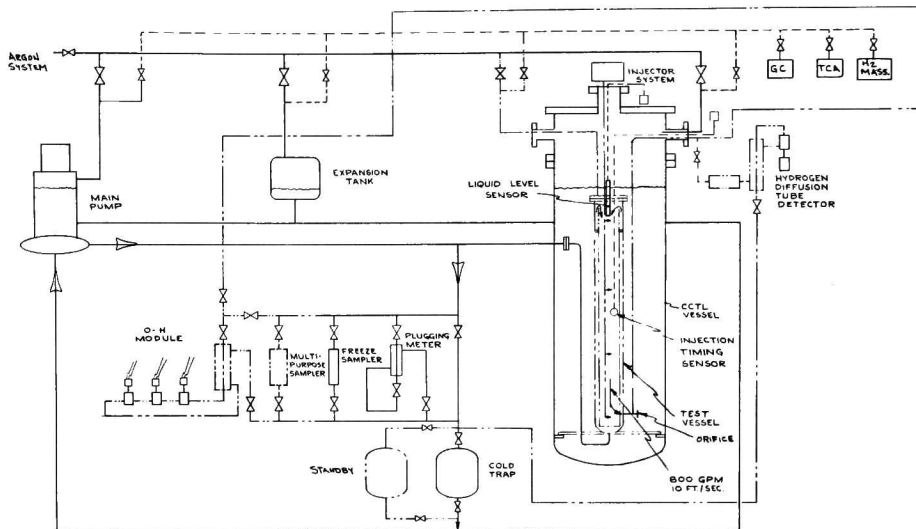


Fig. 1. Schematic Description of CCTL Loop

At several points in the system, sample lines direct a small fraction of the flow to various types of hydrogen and oxygen detectors. Among others, in-sodium hydrogen-diffusion, cover-gas hydrogen-diffusion, and electrochemical-oxygen meters are used. A bypass flow also passes to a purifying system, a cold trap, in which the impurities are removed from the sodium by precipitation. The bypass flows are governed by a series of valves and EM pumps, as shown in Fig. 1.

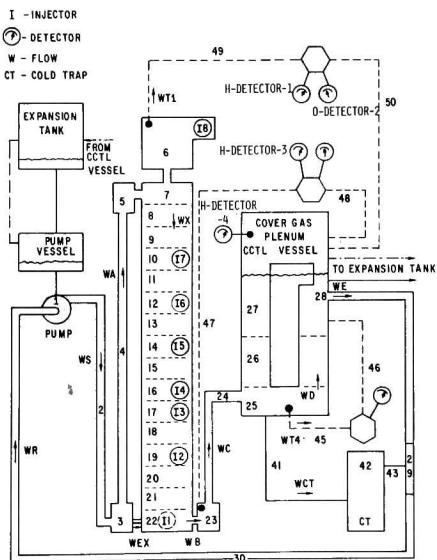


Fig. 2. CCTL Schematics for Simulation Program

A schematic diagram of the CCTL leak-detection experiment, presenting features of importance to the mathematical modeling, is shown in Fig. 2. The CCTL system is divided into segments, each being considered as a lumped-parameter node. Two basic types of segments are used: (1) a mixing plenum, in which ideal mixing is assumed; and (2) pipes in which a pure delay and secondary reactions are assumed.

The steam-generator segments, nodes 6-22, are mixing-plenum segments

each having two baffle plates as a physical boundary. The flow between the segments is forced around the simulated tubes and the periphery of the baffle plate so that the total mixing is a good assumption for these segments. Steam injection points are designated as I1-I8.

Nodes 25-27 are the CCTL vessel segments and contain large volumes of sodium. Node 1 (the pump) and node 27 (the upper vessel section) are in contact with the cover gas, and hydrogen can leave sodium through these segments.

Node 42 is the cold trap where hydrogen and oxygen are removed from the system by cooling and precipitation.

In Fig. 2, detectors are connected to nodes 6, 23, and 25, and the cover-gas plenum; the other nodes depicted are pipe nodes.

The total flow through the system as it leaves the pump is designated as WS; constant flow is assumed. There is a small sodium bypass flow WEX from node 3 to node 22. Flow from node 7 to node 6 is equal to bypass flow WT1 to the detectors connected to pipe node 49. Other flows leaving the main flow are WT3 and WT4, detector flows, and WCT, the cold-trap flow. All bypass flows to the detectors return to the system through upper sodium node 27 in the CCTL vessel. In the version of the program given in Appendix C, up to 50 segments having sodium flow and sodium-water reactions can be simulated.

The CCTL Dynamic Simulation Program (CCTL-DYSP) is based on the above schematic description of the system. The computer code is described in Appendix B. In the program, a mass and concentration balance for each segment shown in Fig. 2 is performed, using the kinetic and the dynamic equations developed in Secs. III and IV.

Simulation of slow transients must include the influence of cold trapping on the hydrogen and oxygen concentration in the system. Details on cold-trap dynamics appear in Sec. V.

Finally, the detector response is simulated by accounting for the hydrogen and oxygen diffusion through the detectors, and the appropriate time delays in the instrumentation piping.

III. THE KINETICS OF SODIUM-WATER INTERACTIONS

A. The Sodium-Water Reactions

When physical contact is made between sodium and water, with an excess of water, a spontaneous violent reaction occurs, producing sodium hydroxide and hydrogen:



However, under small-leak conditions prevailing in steam generators, the ratio of sodium to water is of the order of 10^6 and additional reactions take place:



The relative fraction of water participating in each of these reactions is dependent on the quantity of water introduced by the leak, the sodium temperature, and the sodium pressure. However, no numerical values were reported in the literature as to the quantity of water going into any of the four above reactions.

Therefore, in the present study, it was assumed that the above reactions are instantaneous and the fraction of water associated with each reaction is K_1 , K_2 , K_3 , and K_4 , respectively, and that

$$K_1 + K_2 + K_3 + K_4 = 1. \quad (5)$$

Accordingly, when Q moles of water leak into sodium, four reaction products are generated with the following distribution:

$$Q(0.5 K_1 + K_4) \text{ moles of } \text{H}_2; \quad (6)$$

$$Q(K_1 + K_2) \text{ moles of } \text{NaOH}; \quad (7)$$

$$Q(K_1 + 2K_3) \text{ moles of } \text{NaH}; \quad (8)$$

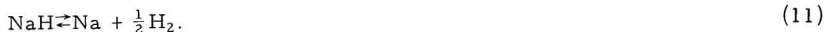
$$Q(K_3 + K_4) \text{ moles of } \text{Na}_2\text{O}. \quad (9)$$

These products are predominantly dissolved and entrained by the rapid turbulent sodium flow. However, a fraction of the hydrogen is entrained as bubbles rather than dissolved in the liquid sodium. These bubbles will either diffuse and dissolve in the fluid, or escape into the cover gas.

Some of the products formed in the primary reactions are unstable at the temperatures prevailing in a steam generator or in the CCTL. The NaH and NaOH are dissociated according to the equations



and



Thus, it is apparent that the ultimate products of the sodium-water reaction are predominantly hydrogen gas and sodium oxide, which can be detected by hydrogen and oxygen meters.

B. Hydrogen Equilibrium Concentration in Sodium

In systems under equilibrium conditions, some of the hydrogen dissolved in sodium escapes to the cover gas and is found to have a partial pressure P_H , independent of the cover gas pressure (usually argon). The equilibrium relation between the hydrogen in the cover gas and hydrogen in sodium (either as hydrogen or as NaH) is governed by the Sieverts' law:⁸

$$C_H = K_S P_H^{1/2}, \quad (12)$$

where C_H is the hydrogen concentration in sodium (in mol/lb) and K_S is Sieverts' constant given by

$$K_S = 2.255 \times 10^{-6} \exp(1.9733 - 276.77/T_K), \quad (13)$$

where K_S is in mol/lb-Torr^{1/2}, T_K is the temperature in degrees Kelvin, and P_H is the hydrogen partial pressure, in Torr (i.e., mm Hg).

C. Decomposition Rate of Sodium Hydroxide

In reactions 1 and 2, sodium hydroxide (NaOH) is formed. This product is unstable under normal reactor operating conditions and decomposes according to Eq. 10. In his experiments, which involved heating sodium with NaOD* at 500°C under vacuum, Fischer⁴ found that the reaction is of the first order according to

$$Rt = \ln[C_0/(C_0 - C)] \quad (14)$$

where C_0 is the initial concentration, C is the concentration at time t , and R is the rate constant.

From the linear portion of the experimental curve, Fischer⁴ determined the rate constant to be

$$R = 0.0045 \text{ min}^{-1},$$

or in other terms, the half-life $\tau_{1/2}$ of NaOH is

*D denotes deuterium.

$$\tau_{1/2} = 150 \text{ min.}$$

Therefore, $K_{\text{NaOH}} = 7.5 \times 10^{-5} \text{ sec}^{-1}$ was used in this study.

The hydroxide decomposition in sodium has also been treated by several authors,^{4,7,10} but none gave the temperature dependence of the reaction rate. In the present study, it was therefore assumed that the reaction rate is a constant.

D. Dissociation Pressure of Sodium Hydride

The partial pressure of hydrogen over NaH has been well established for a wide range of temperatures^{1,4,9} and is given by

$$P_{\text{dis}} = \exp(26.71 - 14046/T_K), \quad (15)$$

where P_{dis} is the dissociation pressure, in mm Hg, and T_K is the temperature, in degrees Kelvin. Banus et al.¹¹ have shown that Eq. 15 is correct, even in dilute sodium solutions; therefore the equation was used in the present study.

E. Hydrogen Absorption by Sodium

Under vacuum conditions at elevated temperatures, all the sodium hydride will be decomposed. However, hydrogen also will be absorbed by sodium if it is available in significant quantities in a cover-gas plenum over the sodium. Experiments by Longton³ reveal that if hydrogen is admitted over sodium at a pressure greater than the dissociation pressure, sodium hydride will form until the pressure decreases to a value equal to the dissociation pressure. The rate of absorption in terms of a pressure change ΔP_H is given by a simple parabolic law

$$\Delta P_H = K(P_H - P_{\text{dis}})^2, \quad (16)$$

where P_H is the actual pressure in the cover gas, P_{dis} is the dissociation pressure, Δ indicates change in the variable, and K is the rate constant, which is temperature-dependent according to the Arrhenius equation

$$K = A \exp(-Q/RT). \quad (17)$$

From the semilogarithmic plots given by Longton,³ A and Q/R have been determined to be

$$A = 1.42 \times 10^9 \text{ sec}^{-1} \text{ and } Q/R = 11795^\circ\text{K.}$$

Note, however, that at the temperatures of interest in the steam generator, the dissociation pressure of NaH is high [for 940°F (504°C), $P_{\text{dis}} = 5670 \text{ mm-Hg}$]; hence, hydrogen from the cover-gas plenum is not expected to be absorbed in sodium.

F. Decomposition Rate of Sodium Hydride

Naud⁶ has reported some experiments to determine NaH dissociation rates. He reported large experimental errors. However, since these are the only rate constants available, they will be used in the present study. The values reported by Naud are

$$K(310^{\circ}\text{C}) = 0.05 \text{ min}^{-1}$$

and

$$K(280^{\circ}\text{C}) = 0.035 \text{ min}^{-1}.$$

On substituting these values into Eq. 17, we obtain the following expression for the rate of NaH dissociation:

$$R_2 = 0.597 \exp(-3883/T_K). \quad (18)$$

If, however, the partial pressure of hydrogen in the cover gas is equal to or greater than the NaH dissociation pressure, there will be no NaH dissociation. It is, therefore, assumed that both processes, i.e., NaH dissociation, and hydrogen absorption by the sodium and formation of sodium hydride, are governed by Eq. 16 and the combined rate constant is given by

$$K_{\text{NaH}} = R_2 \left(\frac{P_{\text{dis}} - P_{\text{H}}}{P_{\text{dis}}} \right)^2. \quad (19)$$

G. Kinetic Equations

In Secs. A-F the various chemical reactions occurring when a small quantity of water is introduced into sodium were described. The dissociation equations of some of the products and their reaction rates were also given.

It is now possible to write the kinetic equations for a volume of sodium into which a leak of Q lb/sec of water has been injected. These equations give the change in concentration of the reaction products as a function of time:

$$\dot{C}_{\text{NaH}} = \frac{d}{dt} C_{\text{NaH}} = (K_2 + 2K_3) \frac{Q}{M} - K_{\text{NaH}} C_{\text{NaH}}, \quad (20)$$

$$\dot{C}_{\text{NaOH}} = \frac{d}{dt} C_{\text{NaOH}} = (K_1 + K_2) \frac{Q}{M} - K_{\text{NaOH}} C_{\text{NaOH}}, \quad (21)$$

$$\dot{C}_{\text{Na}_2\text{O}} = \frac{d}{dt} C_{\text{Na}_2\text{O}} = (K_3 + K_4) \frac{Q}{M} + K_{\text{NaOH}} C_{\text{NaOH}}, \quad (22)$$

and

$$\dot{C}_{H_2} = \frac{d}{dt} C_{H_2} = (0.5K_1 + K_4) \frac{Q}{M} + 0.5(K_{NaH}C_{NaH} + K_{NaOH}C_{NaOH}), \quad (23)$$

where C is the concentration (in mol/lb) of the different products, M is the sodium mass (in lb) in the calculated segment, K_{NaH} is given by Eq. 19, K_{NaOH} is a constant (in sec^{-1}), and Q is the leak rate (in mol/sec).

These equations are used in subsequent sections to develop the dynamic equations used in the simulation study.

IV. DYNAMICS OF SODIUM-WATER REACTION-PRODUCT PROPAGATION

The dynamic equations developed in this section are based mainly on mass balance applied to each segment and each product of the CCTL system. The equations are written in a general way so that the program can be adopted to other systems mainly by changing the input data. Some additional changes may be required due to differences in the physical-loop configurations.

A. Sodium Flow and Concentration Changes

The CCTL system is subdivided into several segment nodes as shown in Fig. 2. In a generalized node, the following processes occur:

1. Primary reactions resulting from water leak.
2. Secondary reactions.
3. Sodium flowing into and out of the segment.
4. Hydrogen gas entering or leaving the node.
5. Precipitation of reaction products.

The appropriate balance equations are

$$\frac{d}{dt} C_1 = \frac{1}{M} \sum_j (W_{ij}C_{1ij} - W_{xj}C_1) + \dot{C}_{NaH}, \quad (24)$$

$$\frac{d}{dt} C_2 = \frac{1}{M} \sum_j (W_{ij}C_{2ij} - W_{xj}C_2) + \dot{C}_{NaOH}, \quad (25)$$

$$\frac{d}{dt} C_3 = \frac{1}{M} \sum_j (W_{ij}C_{3ij} - W_{xj}C_3) + \dot{C}_{Na_2O}, \quad (26)$$

and

$$\frac{d}{dt} C_4 = \frac{1}{M} \sum_j (W_{ij} C_{4ij} - W_{xj} C_4) + \dot{C}_{H_2} - W_H/M, \quad (27)$$

where

$j = 1, \dots, j$ for all inlet and outlet flows,

$i = \text{inlet}$,

$x = \text{exit}$,

$C_1 = \text{concentration of NaH (in mol/lb) at any particular node}$,

$C_2 = \text{concentration of NaOH (in mol/lb) at any particular node}$,

$C_3 = \text{concentration of Na}_2\text{O (in mol/lb) at any particular node}$,

$C_4 = \text{concentration of hydrogen (in mol/lb) at any particular node}$,

$W_{ij} = \text{node inlet flow (in lb/sec) at the } j\text{th inlet}$,

$W_{xj} = \text{node exit flow (in lb/sec) at the } j\text{th outlet}$,

$M = \text{total mass of sodium (in pounds) in the node}$,

$W_H = \text{net hydrogen gas (in mol/sec) leaving (or entering) the node}$,

and

\dot{C}_{NaH} , \dot{C}_{NaOH} , $\dot{C}_{\text{Na}_2\text{O}}$, and \dot{C}_{H_2} are time derivatives given by Eqs. 20, 21, 22, and 23, respectively.

B. Hydrogen Partial Pressure in the Cover Gas

In the sodium loop of an LMFBR steam generator, as well as in the CCTL leak-detection experiment, the sodium may have a free surface with an inert cover gas in several places. Under leak conditions, hydrogen generated in the sodium will escape into the cover gas. If, for some reason, a high concentration of hydrogen or steam exists in the cover gas, it will be partially absorbed in the sodium flow.

In the CCTL experiment, the coolant contacts the cover gas in two places: the pump and the CCTL vessel. The amount of gas (in mol/sec) that can leave these nodes is W_{HP} and W_{HC} for the pump and the CCTL vessel, respectively. All cover-gas plena are connected through the expansion tank, and equal pressure is assumed to exist in each plenum.

The hydrogen partial gas pressure P_H is calculated from the ideal gas law $PV = nRT$:

$$W_H = W_{HP} + W_{HC}; \quad (28)$$

$$\frac{dP_H}{dt} = 554.4 W_H T_{pl} / V_{pl}, \quad (29)$$

where P_H is in mm Hg, W_H is in mol/sec; T_{pl} is the temperature (in degrees Rankine), and V_{pl} is the total plenum volume (in cubic feet).

C. Hydrogen-gas Migration

The quantity of hydrogen gas produced at the leak site is given by Eq. 6. This hydrogen can be in two forms; it can be either dissolved in the sodium or in the form of tiny bubbles. No information was found in the literature on whether any hydrogen bubbles are formed and what the fraction or sizes of these bubbles are. From the experiments performed so far there is, however, a strong indication that no bubbles are formed at the high temperatures prevailing in the heat exchanger, but some of the hydrogen might be produced in bubbles under low-temperature condition.

The conditions under which hydrogen bubbles are formed and their subsequent behavior in the system are the subject of ongoing theoretical and experimental investigations. In this study, it is assumed that if free hydrogen is formed during reactions at the leak site, it will be completely dissolved in the sodium. This assumption is well justified above 600°F (316°C) and will probably be increasingly erroneous as the temperature of the sodium in the CCTL experiment is lowered.

A model for the possible migration or diffusion of the dissolved hydrogen and its subsequent escape into the cover gas has been developed based on the following assumptions:

1. Dissolved hydrogen will diffuse from the sodium into the cover gas only when the partial pressure in the cover gas is less than the value governed by Sieverts' law (Eq. 12).
2. Hydrogen from the cover gas will enter the sodium only if the partial pressure of the cover gas is higher than the NaH dissociation pressure.
3. Independent hydrogen-gas migration occur only in parts of the system where very slow flow exists; otherwise the gas will be entrained in the sodium flow.
4. The gas will migrate only in the upward direction.
5. The rate at which the hydrogen migrates to the cover gas is determined by the difference between hydrogen concentration and the equilibrium value according to Seiverts' law:

$$W_H = R_1(C_H - C_{HS})M \text{ for } C_H > C_{HS}. \quad (30)$$

6. The rate constant R_1 , which governs the hydrogen disengagement rate, is assumed to be such that, if zero partial pressure of hydrogen exists in the cover gas, it will take $\tau_{1/2}$ for half the hydrogen necessary to establish equilibrium to leave the sodium node:

$$R_1 = (\ln 2)/\tau_{1/2} = 0.693/\tau_{1/2}. \quad (31)$$

D. Dynamics of a Pipe Segment

Dynamic equations for a pipe containing M pounds of sodium flowing at W lb/sec are determined by the transit time τ , which is given by

$$\tau = M/W. \quad (32)$$

The concentration of any of the reaction products at time $t - \tau$ is given by

$$C' = C(t - \tau). \quad (33)$$

Hence, C' is the concentration of a reaction product τ seconds before it reaches the pipe exit.

There are no leaks in these pipe segments; therefore, only secondary reactions take place. The change in C' , which was confined to the pipe segment during time τ , is obtained by the following single-step integration process:

$$\Delta C_1 = -K_{NaH}C'_1\tau, \quad (34)$$

$$\Delta C_2 = -K_{NaOH}C'_2\tau, \quad (35)$$

$$\Delta C_3 = K_{NaOH}C'_2\tau, \quad (36)$$

and

$$\Delta C_4 = 0.5(K_{NaH}C'_1 + K_{NaOH}C'_2)\tau. \quad (37)$$

This is a coarse integration process and can be justified only because the secondary reaction-rate constants are very small.

The concentration of any of the reaction products at the exit of the pipe at time t is given by

$$C(t) = C' + \Delta C. \quad (38)$$

V. THE COLD TRAP

Impurities are removed from the sodium by cooling it to temperatures at which the solubility of some of the reaction products is reduced considerably.

A small stream of the sodium is bypassed through a special heat exchanger called a cold trap. If the concentration of the impurities exceeds the amount that can be dissolved in sodium at the cold-trap temperature, the excess will precipitate.

A. Cold-trap Efficiency

Theoretically, the impurity concentration in sodium at the cold-trap outlet should be equal to its solubility at the cold-trap temperature. However, the operating characteristics of the cold trap change with time and flow rate, with consequent changes in its static efficiency, which is given by¹²

$$\beta = \frac{C_i - C_x}{C_i - C_{sat}}, \quad (39)$$

where C_i and C_x are the impurity concentrations at the inlet and outlet, and C_{sat} is the saturation concentration for the cold-trap temperature.

B. Cold-trap Dynamics

In a dynamic system, the widely accepted concept of the static efficiency β cannot be used. Instead, a dynamic efficiency is defined by

$$M \frac{dC}{dt} = W_{ct}(C_{in} - C) - \beta_d(C_{in} - C_{sat}), \quad (40)$$

where C is the average outlet concentration (in mol/lb), and β_d is the dynamic efficiency, given by

$$\beta_d = f(W_{ct}, T_{ct}), \quad (41)$$

where W_{ct} is flow rate through the cold trap (in lb/sec), and M is the sodium content in the cold trap (in pounds). The exact dependence of β_d on the flow rate and other factors is presently unknown.

C. Solubility of Reaction Products

Available data on the solubility of hydrogen and oxygen in sodium have been summarized by Rodgers and Dutina.⁵ Their recommended values as function of temperature were used in this study.

$$\text{For NaH, } C_{1sat} = \exp(13.97 - 6631.4/T_K). \quad (42)$$

$$\text{For Na}_2\text{O, } C_{3sat} = \exp(16.131 - 6493.3/T_K). \quad (43)$$

The concentrations are given in ppm, and T_K is the cold-trap temperature in degrees Kelvin.

VI. DETECTORS

The results of the CCTL leak-detection experiments will be available through reading and interpreting outputs from the hydrogen and oxygen detectors. Outputs from the hydrogen detectors will be proportional to the NaH and hydrogen concentrations, and outputs from the oxygen detectors will be proportional to the Na₂O concentration.

To predict the detector outputs, the simulation employs three parameters that characterize the detectors: (1) the time lag τ , which is the time for the tiny stream of sodium to reach the detecting apparatus; (2) the diffusion time constant θ of the detector, i.e., the time for hydrogen or oxygen to diffuse through the membrane until equilibrium is achieved between the measured sample stream and the detector interior; and (3) the proportionality or calibration constant of the detector.

The detector transfer function is given by

$$\frac{A}{C} = \frac{K_d e^{-S\tau}}{1 + S\theta}, \quad (44)$$

where A is the detector reading, C is the actual concentration, S is the Laplace-transform operator, and K_d is the proportionality constant.

VII. A TYPICAL DATA SET TO BE USED WITH THE SIMULATION

A data set that describes the CCTL system, the conditions at which the particular experiment is performed, and some initial conditions is given in Tables I-VII. Except for the explanatory titles, the tables are reproductions of CCTL-DYSP printouts of initial data used in a CCTL leak-detection-experiment simulation.

Table I presents data describing the system segments, length, cross section, area, the total mass of sodium in each segment, and the flow through each segment. Table II shows the initial conditions in each segment. Table III gives some reaction parameters and how much of each reaction product is generated per mole of water leak. Table IV gives some system constants, and Table V gives the input flow values through various passages. Table VI shows the leak experiment for a particular run, and Table VII describes the detectors.

TABLE I. Description of CCTL Experiment by Segments.

TYPE 0, not simulated; TYPE 1, mixing plenum;
 TYPE 2, a pipe segment; TYPE 3, plenum with cover
 gas; TYPE 4, segment with multiple entry; TYPE 5,
 segment with cover gas and multiple entry.

***** RUN # 24: CCTLP LEAK DETECTION							
SEGM	TYPE	SEGMENT PARAMETERS					
		LENGTH (ft)	CROSS-AREA (ft ²)	MASS (lb)		FLOW (lb/sec)	
1	*	3	1.000E 00	1.069E 00	5.583E 01	9.309E 01	
2	*	2	4.090E 01	9.893E-02	2.113E 02	9.309E 01	
3	*	1	1.000E 00	3.395E-01	1.773E 01	9.309E 01	
4	*	2	1.000E 01	9.893E-02	5.166E 01	9.297E 01	
5	*	1	1.000E 00	2.127E-01	1.111E 01	9.297E 01	
6	*	1	1.000E 00	1.490E 00	7.781E 01	5.818E-01	
7	*	1	2.775E-01	3.240E-01	4.095E 00	9.297E 01	
8	*	1	4.171E-01	3.240E-01	7.057E 00	9.239E 01	
9	*	1	4.021E-01	3.240E-01	6.803E 00	9.239E 01	
10	*	1	4.588E-01	3.240E-01	7.763E 00	9.239E 01	
11	*	1	7.788E-01	3.240E-01	1.318E 01	9.239E 01	
12	*	1	8.546E-01	3.240E-01	1.446E 01	9.239E 01	
13	*	1	7.788E-01	3.240E-01	1.318E 01	9.239E 01	
14	*	1	7.221E-01	3.240E-01	1.222E 01	9.239E 01	
15	*	1	7.221E-01	3.240E-01	1.222E 01	9.239E 01	
16	*	1	7.788E-01	3.240E-01	1.318E 01	9.239E 01	
17	*	1	8.546E-01	3.240E-01	1.446E 01	9.239E 01	
18	*	1	7.788E-01	3.240E-01	1.318E 01	9.239E 01	
19	*	1	4.588E-01	3.240E-01	7.763E 00	9.239E 01	
20	*	1	4.021E-01	3.240E-01	6.803E 00	9.239E 01	
21	*	1	4.171E-01	3.240E-01	7.057E 00	9.239E 01	
22	*	4	3.889E-01	3.240E-01	6.580E 00	9.251E 01	
23	*	1	1.000E 00	2.127E-01	1.111E 01	9.251E 01	
24	*	2	2.890E 00	9.893E-02	1.493E 01	9.192E 01	
25	*	1	1.000E 00	4.030E 00	2.105E 02	9.192E 01	
26	*	1	2.083E 00	6.335E 00	0.691E 02	9.146E 01	
27	*	5	7.500E 00	0.445E 00	2.524E 03	9.262E 01	
28	*	2	1.900E 01	1.525E-01	1.514E 02	9.262E 01	
29	*	4	8.000E-01	1.525E-01	0.573E 00	9.309E 01	
30	*	2	3.100E 01	1.525E-01	2.470E 02	9.309E 01	
31	*	0	1.000E 00	0.0	0.0	0.0	
32	*	0	1.000E 00	0.0	0.0	0.0	
33	*	0	1.000E 00	0.0	0.0	0.0	
34	*	0	1.000E 00	0.0	0.0	0.0	
35	*	0	1.000E 00	0.0	0.0	0.0	
36	*	0	1.000E 00	0.0	0.0	0.0	
37	*	0	1.000E 00	0.0	0.0	0.0	
38	*	0	1.000E 00	0.0	0.0	0.0	
39	*	0	1.000E 00	0.0	0.0	0.0	
40	*	0	1.000E 00	0.0	0.0	0.0	
41	*	2	2.800E 01	2.480E-03	3.626E 00	4.654E-01	
42	*	1	1.000E 00	3.276E 00	1.711E 02	4.654E-01	
43	*	2	1.600E 01	2.480E-03	2.072E 00	4.654E-01	
44	*	0	1.600E 01	1.796E-01	1.501E 02	0.0	
45	*	0	0.0	0.0	0.0	0.0	
46	*	0	0.0	0.0	0.0	0.0	
47	*	2	1.858E 01	2.480E-03	2.407E 00	5.818E-01	
48	*	2	3.687E 01	2.480E-03	7.182E 00	5.818E-01	
49	*	2	4.267E 01	2.480E-03	5.526E 00	5.818E-01	
50	*	2	4.226E 01	2.480E-03	1.100E 01	5.818E-01	

TABLE II. Initial Concentration of Reaction Products
in Different Segments of CCTL

SEGM	TYPE	CONCENTRATION, MOL/LB				
		C1-NAH	C2-NAOH	C3-NA2O	C4-H2	
1	*	3	1.418E-06	1.134E-08	2.561E-04	2.249E-06
2	*	2	1.418E-06	1.134E-08	2.561E-04	2.249E-06
3	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
4	*	2	1.418E-06	1.134E-08	2.561E-04	2.249E-06
5	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
6	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
7	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
8	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
9	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
10	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
11	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
12	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
13	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
14	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
15	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
16	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
17	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
18	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
19	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
20	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
21	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
22	*	4	1.418E-06	1.134E-08	2.561E-04	2.249E-06
23	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
24	*	2	1.418E-06	1.134E-08	2.561E-04	2.249E-06
25	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
26	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
27	*	5	1.418E-06	1.134E-08	2.561E-04	2.249E-06
28	*	2	1.418E-06	1.134E-08	2.561E-04	2.249E-06
29	*	4	1.418E-06	1.134E-08	2.561E-04	2.249E-06
30	*	2	1.418E-06	1.134E-08	2.561E-04	2.249E-06
31	*	0	0.0	0.0	0.0	0.0
32	*	0	0.0	0.0	0.0	0.0
33	*	0	0.0	0.0	0.0	0.0
34	*	0	0.0	0.0	0.0	0.0
35	*	0	0.0	0.0	0.0	0.0
36	*	0	0.0	0.0	0.0	0.0
37	*	0	0.0	0.0	0.0	0.0
38	*	0	0.0	0.0	0.0	0.0
39	*	0	0.0	0.0	0.0	0.0
40	*	0	0.0	0.0	0.0	0.0
41	*	2	1.418E-06	1.134E-08	2.561E-04	2.249E-06
42	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
43	*	2	1.418E-06	1.134E-08	2.561E-04	2.249E-06
44	*	0	0.0	0.0	0.0	0.0
45	*	0	0.0	0.0	0.0	0.0
46	*	0	0.0	0.0	0.0	0.0
47	*	2	1.418E-06	1.134E-08	2.561E-04	2.249E-06
48	*	2	1.418E-06	1.134E-08	2.561E-04	2.249E-06
49	*	2	1.418E-06	1.134E-08	2.561E-04	2.249E-06
50	*	2	1.418E-06	1.134E-08	2.561E-04	2.249E-06

TABLE III. Leak Distribution to Various Reactions and Reaction Products

0.45 OF THE LEAK GOES TO	$\text{NA} + \text{H}_2\text{O} = \text{NAOH} + 1/2\text{H}_2(\text{G})$
0.20 OF THE LEAK GOES TO	$2\text{NA} + \text{H}_2\text{O} = \text{NAOH} + \text{NAH}$
0.25 OF THE LEAK GOES TO	$4\text{NA} + \text{H}_2\text{O} = 2\text{NAH} + \text{NA}_2\text{O}$
0.10 OF THE LEAK GOES TO	$2\text{NA} + \text{H}_2\text{O} = \text{NA}_2\text{O} + \text{H}_2$
0.70 MOL OF THE LEAK IS TRANSFORMED TO	NAH
0.65 MOL OF THE LEAK IS TRANSFORMED TO	NAOH
0.35 MOL OF THE LEAK IS TRANSFORMED TO	NA ₂ O
0.32 MOL OF THE LEAK IS TRANSFORMED TO	H ₂ (G)

TABLE IV. Some Constant Parameters of the System

THE NAH DISSOCIATION PRESSURE IN MM-HG IS	5332.611
SODIUM TEMPERATURE IN (DEG-F) IS	900.00
SODIUM TEMPERATURE IN (DEG-K) IS	755.22
SODIUM DENSITY IN (LBS/CUF) IS	52.22
TOTAL WEIGHT OF SODIUM IN THE SYSTEM (LB)	4785.61
COVER GAS PLENUM VOLUME (CUF)	40.00
COLD TRAP DYNAMIC EFFICIENCY (1/SEC) IS	0.2449E-02
NAH SATURATION CONC. AT COLD TRAP (MUL/LB)	0.8542E-06
NA ₂ O SATURATION CONC. AT COLD TRAP (MUL/LB)	0.4096E-05
TOTAL TRANSIT TIME IN CCTL (SEC) IS	46.87
COLD TRAP TEMPERATURE IN (DEG-K) IS	388.56
SIEVERTS CONSTANT IN (MUL/(LB*TOUR**2))	0.1125E-02
PARTIAL HYDROGEN PRESSURE IN COVER GAS (MM-HG)	0.1
PARTIAL ARGON PRESSURE IN COVER GAS (MM-HG)	800

TABLE V. Flow Distribution in CCTL
(see Fig. 2 for explanation)

TOTAL SODIUM FLOW IN (LBS/SEC) IS	93.0872
WCT	0.4654
WT1	0.5818
WT2	0.0
WT3	0.5818
WT4	0.0
WEX	0.1164
WA	92.9709
WX	92.3891
WB	92.5054
WC	91.9236
WD	91.4582
WE	92.6217
WR	93.0872

TABLE VI. Water-leak Description for Experiment 1 Run 24

*****RUN # 15: CCTL LEAK DETECTION SIMULATION.(.001LB/SEC AT INJ#4, DUR=70SEC*****

LEAKAGE DATA FOR THIS CASE ARE:

FOR NODE SEGMENT #	22	19	17	16	15	12
THE LEAKAGE IN MOL/SEC IS	0.0	0.0	0.0	0.3776E 00	0.0	0.0
THE LEAK STARTS AT TIME -	10.00	10.00	10.00	10.00	10.00	10.00
THE LEAK IS TERMINATED AT	80.00	80.00	80.00	15.00	80.00	80.00

TABLE VII. Description of Detector Connections for Experiment 1 Run 24

DETECTOR NO 1 OF TYPE 1 IS CONNECTED TO NODE 49 HAS A LAG OF 10.00SEC AND A DELAY OF 14.00SEC
 DETECTOR NO 2 OF TYPE 2 IS CONNECTED TO NODE 49 HAS A LAG OF 12.00SEC AND A DELAY OF 15.00SEC
 DETECTOR NO 3 OF TYPE 1 IS CONNECTED TO NODE 47 HAS A LAG OF 10.00SEC AND A DELAY OF 14.00SEC
 DETECTOR NO 4 OF TYPE 3 IS CONNECTED TO NODE 27 HAS A LAG OF 1.00SEC AND A DELAY OF 10.00SEC

Type 1 = Hydrogen Detector

Type 2 = Oxygen Detector

Type 3 = Hydrogen Detector in the Cover Gas

VIII. SUMMARY OF ASSUMPTIONS

1. Reactions 1-4 are the only sodium-water reactions expected at the leak site.
2. As a result of a leak of 1 mol of water, the following reaction products will be generated instantaneously:

0.7 mol of NaH

0.65 mol of NaOH

0.35 mol of Na_2O

0.37 mol of H_2

3. The only secondary reactions taking place in the system are NaOH and NaH dissociation, as given by Eqs. 10 and 11.
4. The half-life of NaOH is 150 min.
5. The NaH dissociation pressure is given by Eq. 15:

$$P_{\text{dis}} = \exp(26.71 - 14046/T_K).$$

6. If the system is at steady state for a long time, the hydrogen pressure in the cover gas will be in equilibrium with the hydrogen concentration in the sodium according to Sieverts' law.
7. Changes in the cover-gas hydrogen partial pressure are the result of hydrogen leaving the sodium according to the Sieverts' law and because of bubble transport from the leak site. Bubble transport occurs only at low temperatures and is assumed to be zero at the temperatures considered in this study.
8. The NaH dissociation rate is given by

$$K_2 = 0.597 \exp(-3883/T_K) \left(\frac{P_{\text{dis}} - P_H}{P_{\text{dis}}} \right)^2.$$

9. Ideal mixing is assumed in all plenum segments.
10. Hydrogen diffusion through the system walls is neglected.
11. The hydrogen and oxygen detectors are of the diffusion type and can be characterized by the transfer function given in Eq. 44:

$$\frac{A}{C} = \frac{K_d e^{-S\tau}}{1 + S\theta}.$$

12. Solubility of NaH in sodium is given by Eq. 42,

$$C_{\text{NaH}} = \exp(13.97 - 6631.4/T_K).$$

13. Solubility of Na₂O in sodium is given by Eq. 43,

$$C_{\text{Na}_2\text{O}} = \exp(16.131 - 6493.3/T_K).$$

14. Steady-state flow conditions prevail throughout the system; therefore, there is a constant sodium level in CCTL vessel and zero flow to the expansion tank.
15. The system temperature is constant; no heat transfer is accounted for.
16. Pressure gradients throughout the flow path and their possible effects on reaction rates are neglected.

IX. SAMPLE CALCULATIONS

The following sample calculations are intended to demonstrate various output features of the program rather than to predict the results of a particular CCTL experiment.

A. Changes in Reaction-product Concentration as a Result of a Short, 0.075-lb Leak

A short leak of 0.015 lb/sec, starting at 10 sec after simulation startup and terminating at 15 sec, was generated to initiate a transient in the CCTL system. The injection point was I4 (in the middle of the steam-generator module). The conditions are basically similar to those given in Tables I-VII, except for the leak size. The simulation was run for 100 sec, a sufficient time for the major transients to be terminated.

Figure 3 shows the hydrogen concentration in sodium as a function of time (1) at the leak-injection site (node 16); (2) at the stagnant part of the steam generator (node 6) through which there is a small (5-gal/min) sampling-line flow; (3) at the end of the pipe leading to hydrogen detector No. 1; and (4) as given by the response of detector No. 1. The delays among the various nodes are clearly visible. The effect of mixing increases with distance from the injection node; therefore, the peaks observed during the transients are lower at the distant nodes.

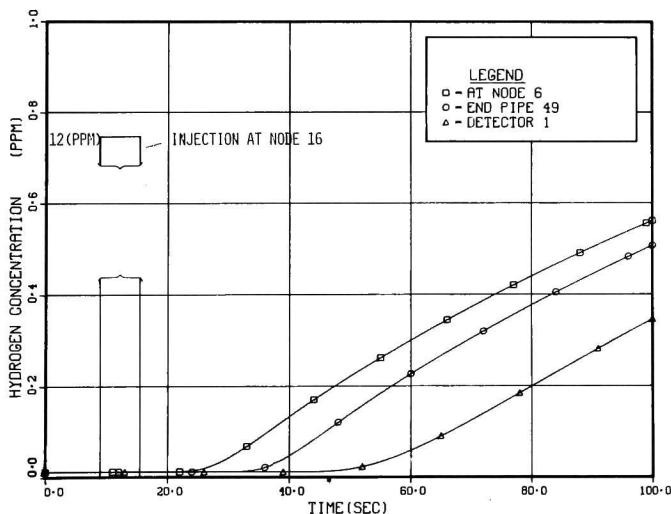


Fig. 3. Transient Hydrogen Concentrations at Node 6, End of Pipe 49, in Detector 1, Resulting from a Steam Injection of 0.015 lb/sec for 5 sec from Injector I4 at Node 16 (See Fig. 2)

Figure 4 shows the hydrogen concentration (1) at the steam-generator outlet plenum (node 23); (2) at the end of sampling line 47 leading from node 23 to the hydrogen detector No. 3; and (3) as given by the response of detector No. 3. For comparative purposes, the hydrogen concentration at the injection node is also shown.

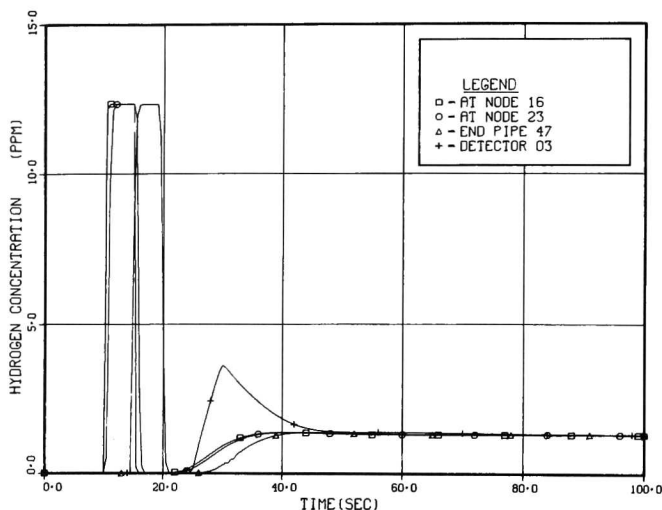


Fig. 4. Transient Hydrogen Concentrations at Nodes 16 and 23, End of Pipe 47, in Detector 3, Resulting from a Steam Injection of 0.015 lb/sec for 5 sec from Injector I4 at Node 16 (See Fig. 2)

Figure 5 shows the concentration of the four reaction products at node 27, which is in contact with the cover gas. Apart from differences in concentrations, which are the results of the assumption on how the sodium-water reaction products split, the transient forms of the four curves are identical.

Figure 6 shows the oxygen concentration at node 6, as monitored by oxygen detector No. 2.

B. Changes in Reaction-product Concentration as a Result of a 70-sec, 0.0001-lb/sec Leak

This run simulated a proposed CCTL leak-detection experiment with a sodium flow rate of 800 gal/min at 940°F (504°C). Steam at 0.001 lb/sec was introduced at Injector I4 (see Fig. 2) 10 sec after simulation startup. The leak was terminated at 80 sec, and simulation was continued up to 600 sec. The cold trap was not in operation in this experiment.

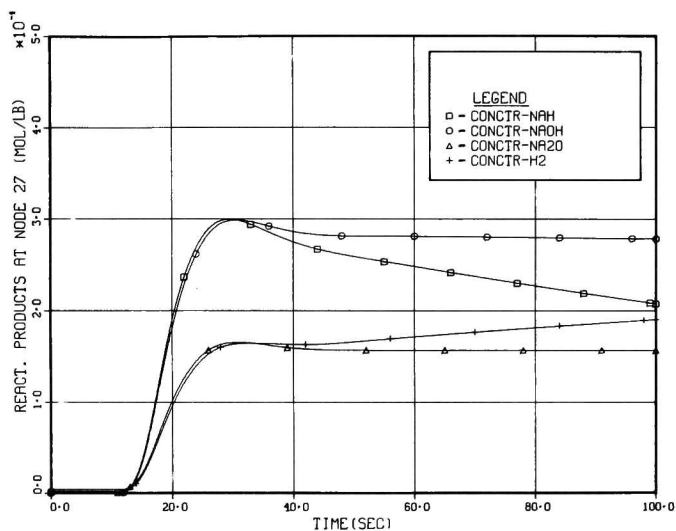


Fig. 5. Transient Concentrations of Reaction Products Resulting from Steam In-
jection of 0.015 lb/sec for 5 sec from Injector I4 at Node 16 (See Fig. 2)

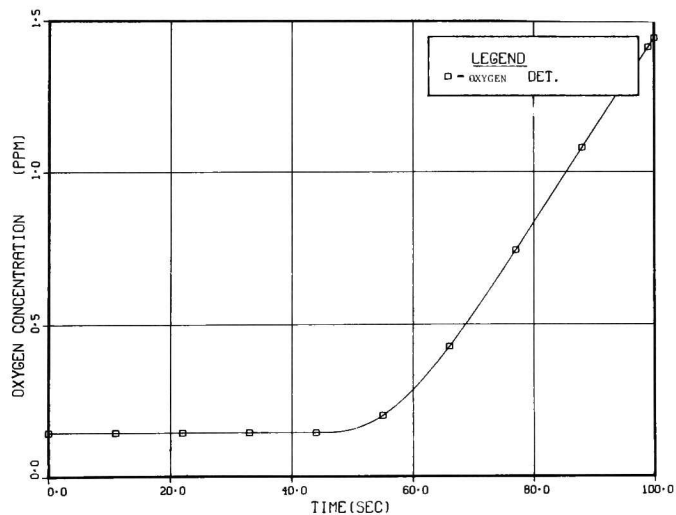


Fig. 6. Oxygen Concentration at Node 6 as Monitored by Oxygen
Detector No. 2 Resulting from Steam Injection of 0.015 lb/
sec for 5 sec at Injector I4 (See Fig. 2)

Figure 7 shows the hydrogen concentration at the injection point (node 16), at node 23, at the end of pipe section 47, and at hydrogen detector No. 3. The delays in concentration changes among the various nodes are clearly seen.

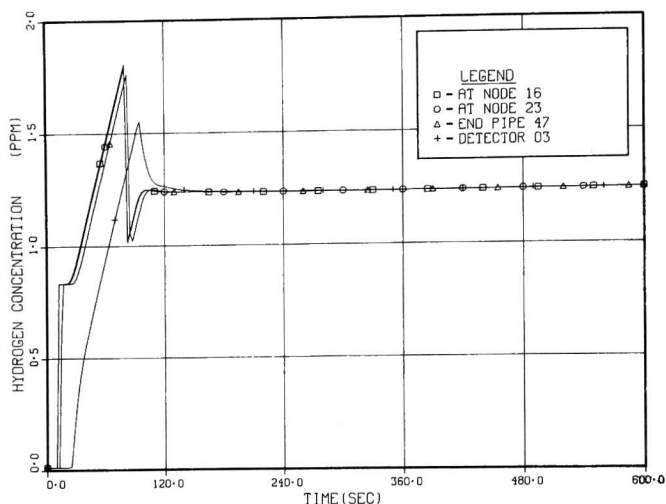


Fig. 7. Transient Hydrogen Concentrations at Nodes 16 and 23, End of Pipe 47, in Detector 3, Resulting from a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4 and Node 16 (See Fig. 2); Sodium Flow Rate of 800 gal/min at 940°F (504°C), without Cold Trapping

Figure 8 shows the concentrations of the four reaction products at node 27. A relatively fast decomposition of NaH at 940°F (504°C) can be observed from the figure.

Figure 9 shows the responses of two hydrogen detectors, one monitoring node 6 and the other monitoring node 23.

Figure 10 shows the hydrogen concentration at the injection node 16, the pump node 1, and the upper CCTL vessel node 27. Except for the time scale, these results are similar to those calculated by Pellow.¹²

C. Effect of Changing Flow Rate

As mentioned earlier, the CCTL test plan¹ includes experiments to determine hydrogen-detector response to steam injections into sodium at various flow rates. Simulations of these experiments consisted of introducing steam at 0.001 lb/sec for 70 sec at node 16 into sodium at 300, 465, 630, and 800 gpm.

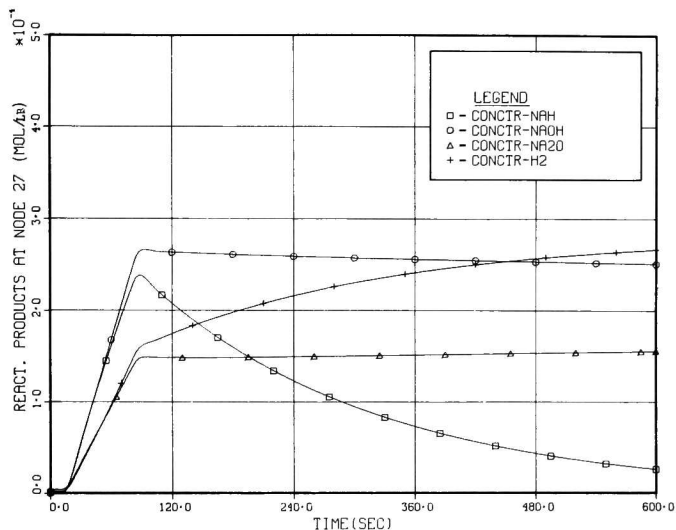


Fig. 8. Transient Concentrations of Reaction Products Resulting from a Steam* Injection of 0.001 lb/sec for 70 sec at Injector I4; Sodium Flow Rate of 800 gal/min at 940°F (504°C), without Cold Trapping

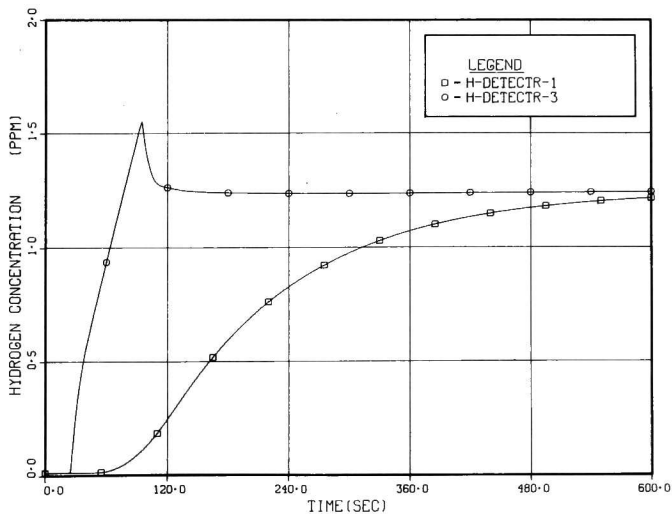


Fig. 9. Response of Hydrogen Detectors to a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4 (See Fig. 2); Sodium Flow Rate of 800 gal/min at 940°F (504°C), without Cold Trapping

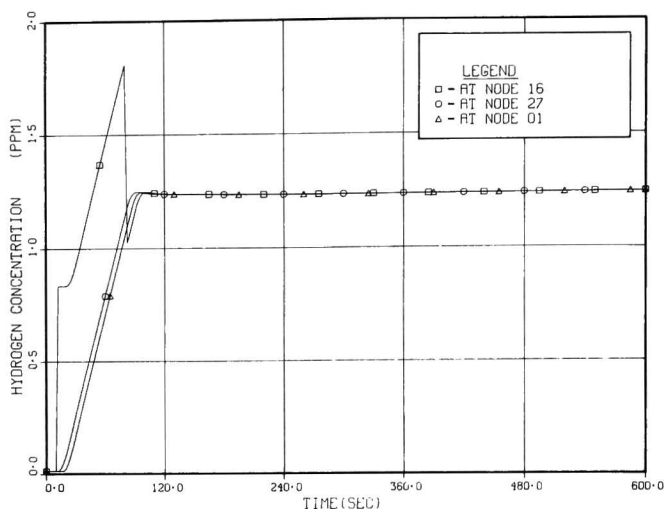


Fig. 10. Transient Hydrogen Concentrations at Nodes 1, 16, and 27 Resulting from a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4 (See Fig. 2); Sodium Flow Rate of 800 gal/min at 940°F (504°C), without Cold Trapping

Figure 11 shows the response of hydrogen detector No. 1 (see end of pipe 49, Fig. 2), which monitored the upper stagnant-sodium section of the steam-generator module during sodium flow rates of 300 and 800 gpm.

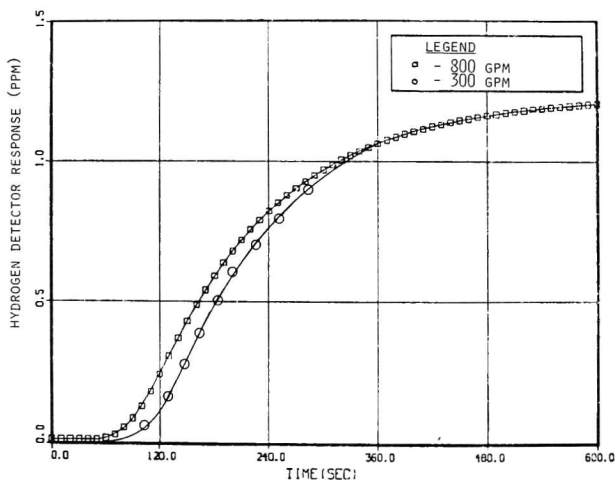


Fig. 11. Response of Hydrogen Detector No. 1 (See Fig. 2) at Different Sodium Flow Rates, to a Steam Injection of 0.001 lb/sec for 70 sec from Injector I4

Figures 12-15 show the response of hydrogen detector No. 3, which monitored the steam-generator outlet during sodium flow rates of 300, 465, 630, and 800 gpm, respectively.

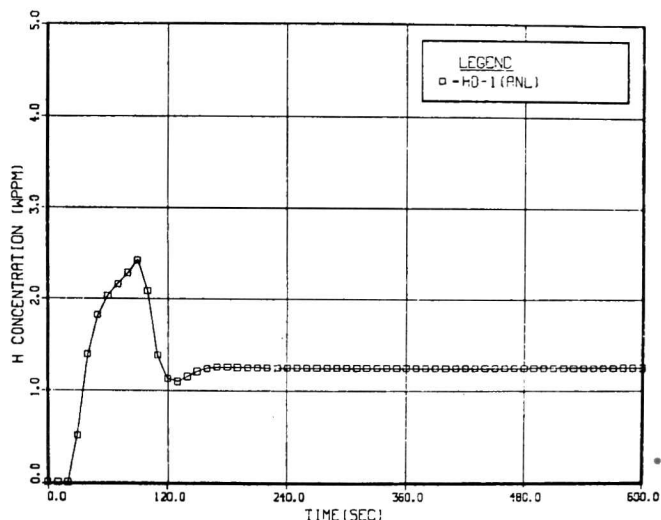


Fig. 12. Response of Hydrogen Detector No. 3 to a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4, during Sodium Flow at 300 gpm

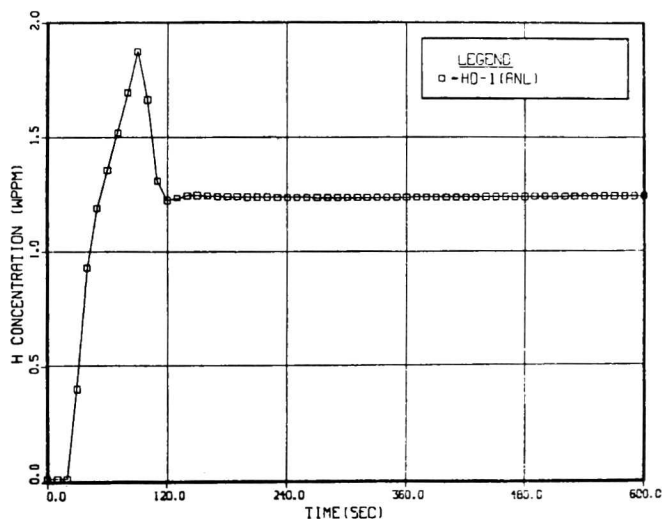


Fig. 13. Response of Hydrogen Detector No. 3 to a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4, during Sodium Flow at 465 gpm

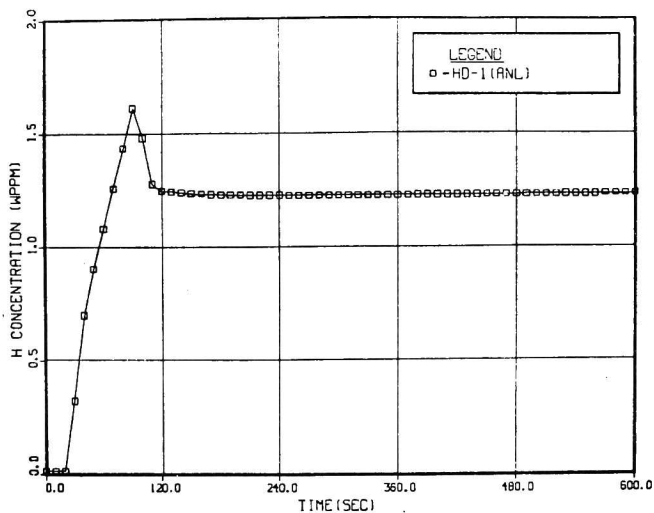


Fig. 14. Response of Hydrogen Detector No. 3 to a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4, during Sodium Flow at 630 gpm

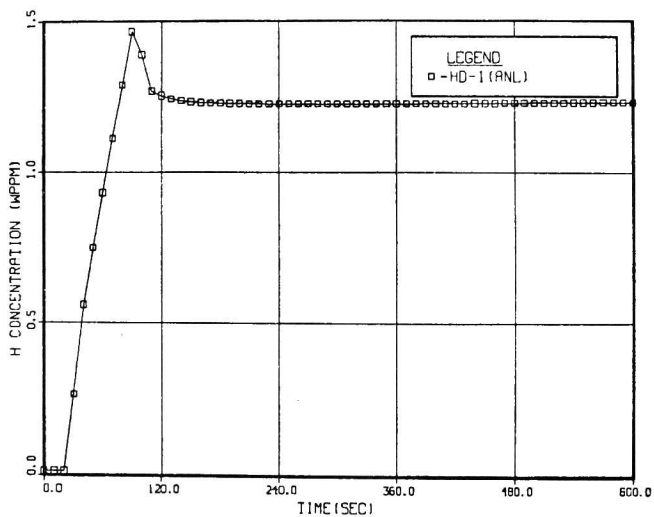


Fig. 15. Response of Hydrogen Detector No. 3 to a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4, during Sodium Flow at 800 gpm

These figures reveal that the delay between leak occurrence and detection of hydrogen concentration increases as the flow rate is decreased. If the detector is close to the leak site, as with, for example, detector number 3 in this case, the maximum transient overshoot in detector response increases when flow rate is reduced.

D. Simulation of a Tightly Coupled Loop

The flexibility of the program is demonstrated by simulating a different type of loop. In this system, the huge sodium vessel containing the steam generator is excluded. Instead, three more segments are added to the steam generator unit. A short leak of 0.015 lb/sec for a 5-sec period was injected from Injector I4 at 800 gpm and was simulated at 940°F (504°C). The results are shown in Figs. 16-20.

The oscillatory nature of the concentration changes is due to the elimination of the huge mixing volumes of the CCTL vessel, which smooth out any type of transient. A short leak, such as is simulated in this experiment, will contaminate a lump of sodium. Whenever this lump passes through a segment of the loop or near a detector, an increase in contamination is observed. After several passages, the transients die out because of the mixing process. The distance between the peaks in the figures is the transit time and is observed to be 14 sec (calculated value, 13.76 sec).

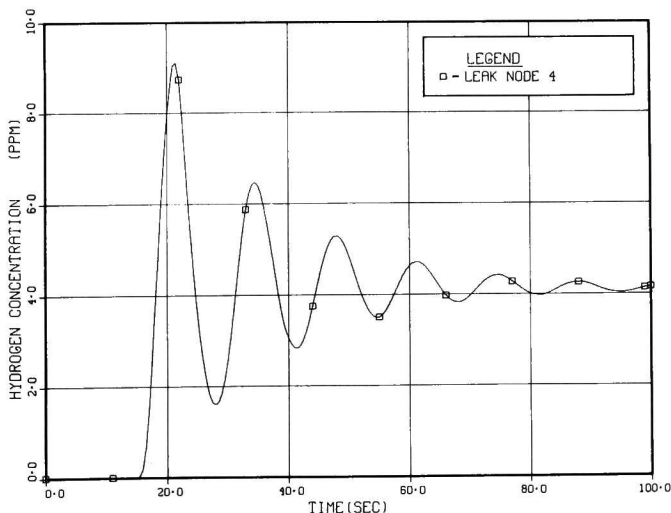


Fig. 16. Transient Hydrogen Concentration in a Tightly Coupled Loop at Pump Node 1 Resulting from a Steam Injection of 0.015 lb/sec for 5 sec into Sodium at 800 gpm and 940°F (504°C), at Injector I4

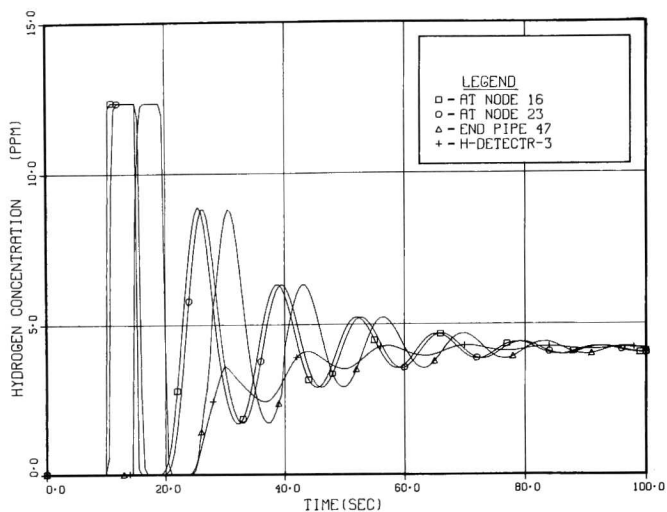


Fig. 17. Transient Hydrogen Concentrations in a Tightly Coupled Loop Resulting from a Steam Injection of 0.015 lb/sec for 5 sec at Injector I4, at 800 gpm and 940°F (504°C)

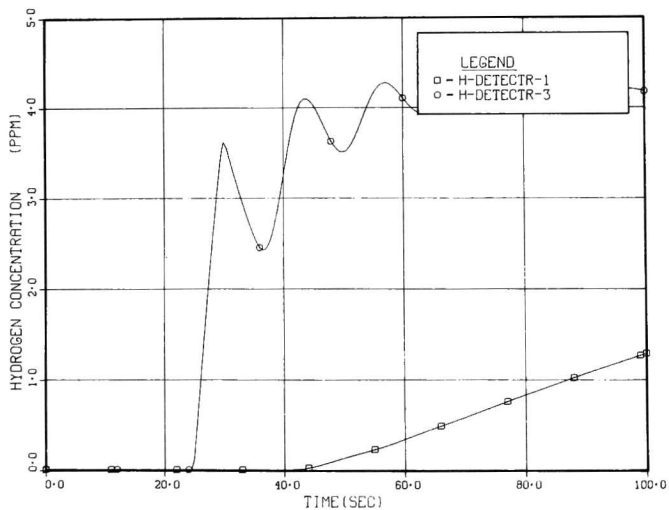


Fig. 18. Response of Hydrogen Detectors in a Tightly Coupled Loop Resulting from a Steam Injection of 0.015 lb/sec for 5 sec at Injector I4, Sodium flow is 800 gpm at 940°F (504°C).

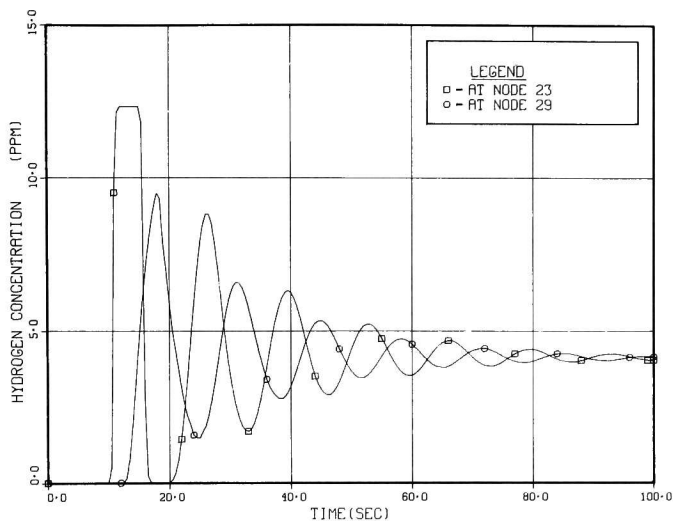


Fig. 19. Transient Hydrogen Concentrations in a Tightly Coupled Loop Resulting* from a Steam Injection of 0.015 lb/sec for 5 sec at Injector I4. Sodium flow is 800 gpm at 940°F (504°C).

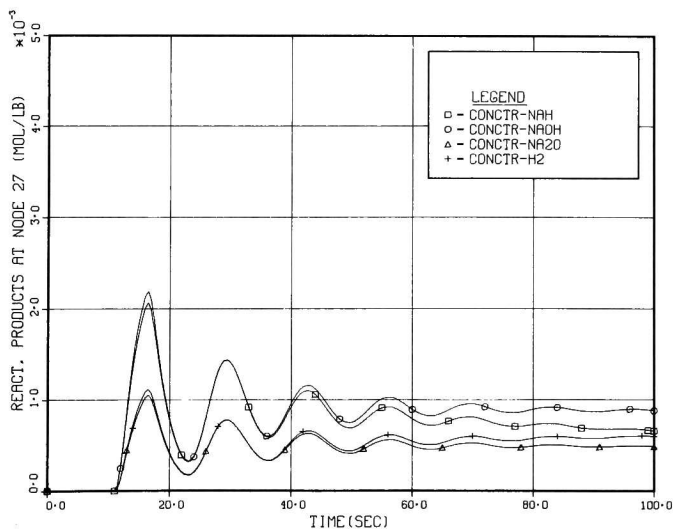


Fig. 20. Transient Concentrations of Reaction Products in a Tightly Coupled Loop Resulting from a Steam Injection of 0.015 lb/sec for 5 sec at Injector I4. Sodium flow is 800 gpm at 940°F (504°C).

Similar results were obtained by Berault et al.,¹³ when a short burst of water was injected into their loop, which included mainly piping segments. The transit time was about 5 min, and 13 peaks were observed before the hydrogen diffused and mixed through system and a stable hydrogen concentration was established.

With reference to the present simulation, Fig. 16 shows the hydrogen concentration at the pump (node 1). Seven peaks occur during the first 100 sec, and the transient dies out soon thereafter.

Figure 17 compares the transient hydrogen concentrations at node 23, end of pipe 47, and the response of detector No. 3 with the transient concentration at the leaking node 16. The leak is represented by a step function 5 sec wide, after which the concentration is reduced to the background value, successive peaks appear after each transit time.

Figure 18 shows the response of hydrogen detectors No. 1 and 3. The integrating effect of the detectors compared to actual hydrogen concentration at nodes 23 and 6 is apparent.

Figure 19 shows the transient hydrogen concentration at nodes 23 and 29. Node 29 is at a "5-sec distance" from node 23. The same transient results; however, because of mixing effects, the appropriate peaks at node 29 are lower than those at segment 23.

Finally, Fig. 20 shows changes in concentration of reaction products NaH, NaOH, Na₂O, and hydrogen at node 27.

E. Effect of Cold-trap Operation

In these simulations, it was assumed that the CCTL cold trap had a static efficiency of $\beta = 0.9$, and the flow through the cold trap was 4 gal/min. Steam was introduced at Injector I4 (node 16), at a rate of 0.0001 lb/sec for 70 sec, and the simulations continued for 15 min. The results with and without cold-trap operation are shown in Figs. 21-24.

Figure 21 shows hydrogen concentrations at node 1, the pump segment. Figure 22 shows the hydrogen concentrations at node 27. Figure 23 gives the response of the hydrogen meter monitoring the steam-generator outlet. Figure 24 shows the Na₂O concentration at node 27.

These results evidence how cold-trap operation reduces impurity concentrations and is reflected in the detector readings. To obtain the new steady-state concentrations resulting from continuous cold-trap operation, the simulation would have had to be continued for about 3 hr. Due to current computer limitations, this was not considered practical. The CCTL-DYSP program has a ratio of simulation time to real time ranging from 0.2 to 0.9. For very fast rates of change in the variables and short transients, the 0.9 ratio should be taken; for slow transients and long simulation times, the 0.2 ratio can be used.

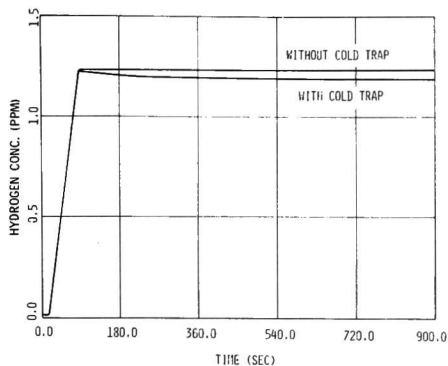


Fig. 21. Effect of Cold-trap Operation on Hydrogen Concentration in the Pump Segment (Node 1)

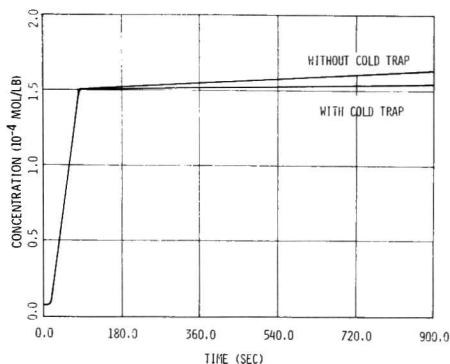


Fig. 22. Effect of Cold-trap Operation on Hydrogen Concentration in the CCTL Vessel (Node 27)

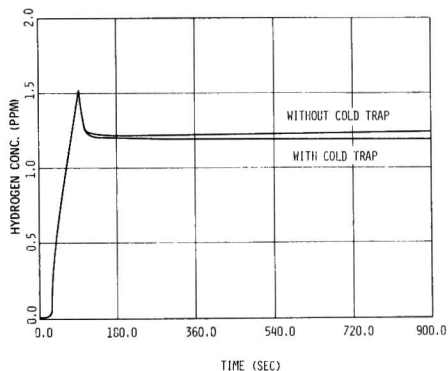


Fig. 23. Effect of Cold-trap Operation on Hydrogen Detector Monitoring the Steam-generator Outlet

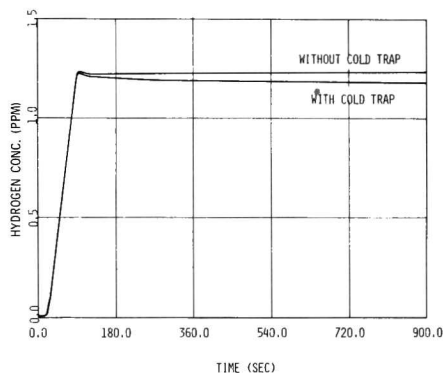


Fig. 24. Effect of Cold-trap Operation on Na₂O Concentration in the CCTL Vessel (Node 27)

F. Effect of Different Reaction Rates

As explained previously (see Sec. III.A, C, and F), little is known about the reaction rates of the various processes occurring once the impurities enter the sodium. It is evident that simulation results cited in previous paragraphs will vary according to the assumptions made concerning the various reaction parameters. For example, the rate at which hydrogen gas leaves the sodium and enters the cover gas will be considered. It is currently assumed that the half-life of hydrogen gas--to reach equilibrium with the cover gas--is 2000 min. At this rate of hydrogen disengagement, no change in the hydrogen content in the cover gas is observed. However, if this half-life is reduced to 2 min, the

hydrogen concentration in the cover gas rises sharply, as shown in Fig. 25. At least some of the uncertainties in these data are expected to be resolved by the CCTL leak-detection experiments.

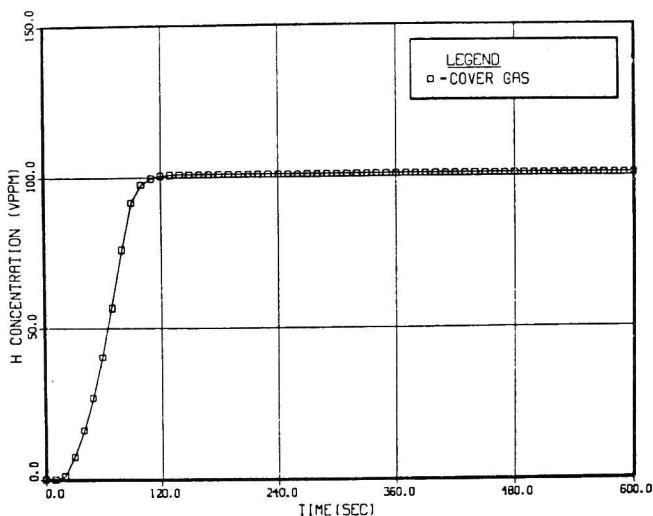


Fig. 25. Change in Cover-gas Hydrogen Concentration When Hydrogen-disengagement Half-life is Reduced by a Factor of 1000

G. Effect of Leak Location

The response of the CCTL experiment detector is expected to vary with the water-leak location. These changes are demonstrated in Figs. 26 and 27, which show the detector response to identical steam injections of 0.01 lb/sec for 5 sec. One injection is close to the steam-generator inlet, Injector I7; the other, Injector I1 is at the steam-generator outlet. Hydrogen detector No. 3 is monitoring the outlet from the steam-generator module. In Fig. 26, the second leak--close to the outlet--is detected first. Figure 27 shows the changes in hydrogen concentration at node 27 resulting from water injected at Injectors I1 and I7.

X. EXPERIMENTAL VERIFICATION

Recently some experimental results from the CCTL leak-detection experiment became available. On November 6, 1975, injection No. 22 took place in which 2.54 g/min of steam were injected at Injector I4. The leak duration was 57.5 sec, the sodium flow was 600 gpm, and the sodium temperature was 940°F (504°C). In Fig. 28 the experimental readings from the hydrogen

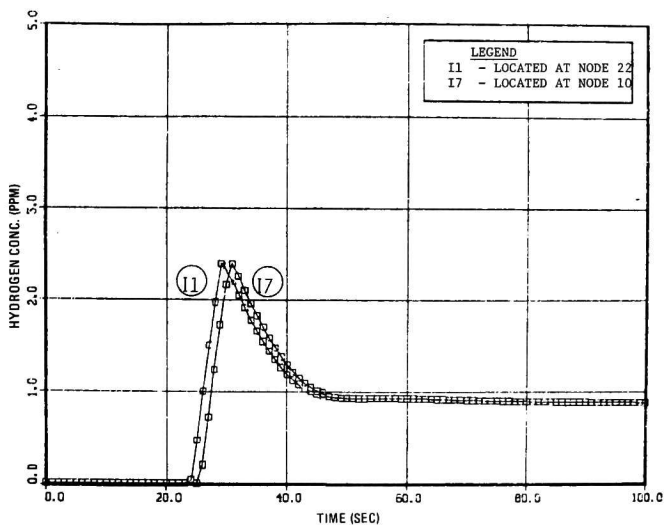


Fig. 26. Response of Hydrogen Detector No. 3 to a Steam Injection of 0.01 lb/sec for 5 sec from Two Different Injectors

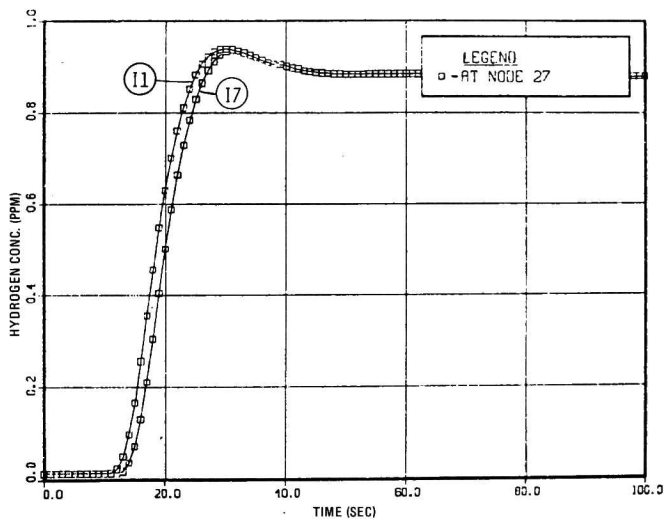


Fig. 27. Transient Hydrogen Concentrations Resulting from Steam Injection of 0.01 lb/sec for 5 sec from Two Different Injectors

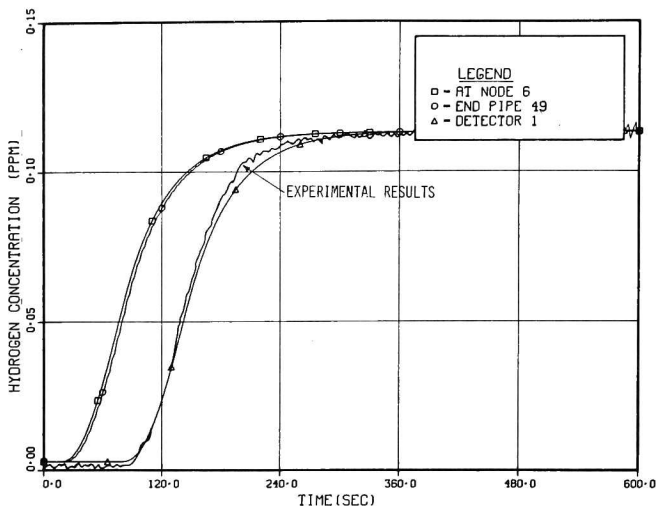


Fig. 28. Effect of Cold-trap Operation on Na_2O Concentration in CCTL Vessel (Node 27)

detector connected to segment 49 are superimposed on the detector response as predicted by the simulation program CCTL-DYSP. Except for random experimental noise, there is excellent agreement. Also shown are the predicted hydrogen concentrations at the end of pipe segment 40, and in the stagnant region of the heat exchanger (segment 6).

On November 7, 1975, injection No. 23 took place in which 0.98 g/min of steam was injected at Injector 14. The leak duration was 118.4 sec, the sodium flow was 300 gpm, and the sodium temperature was 940°F (504°C). In Fig. 29 the experimental readings from the hydrogen detector are superimposed on the detector response as predicted by the simulation. Small differences between the experimental and the predicted curves can be seen. These seem to be mainly due to the imperfect knowledge of the exact shape of the steam-injection curve, errors in the calculation of the delays in the sampling lines due to errors in the flowmeters, and random experimental noise, which is clearly visible on the experimental curve. In this experiment there was apparently a large calibration error in the interpretation of the detector readings. Therefore the experimental results were normalized to the steady-state result as obtained from the simulation.

XI. SUMMARY AND CONCLUSIONS

An analytical model has been developed to describe the kinetic and dynamic processes that occur when water leaks into a circulating sodium loop.

A computer code, CCTL-DYSP, solving the model equations was prepared. The distribution and the concentration of the sodium-water reaction products throughout the system was calculated, and it is shown that qualitatively the results are in agreement with similar calculations or experiments published elsewhere.^{12,13} Subsequent calculations, simulating two CCTL experiments were in good agreement with measured hydrogen concentrations (see Sec. X). However, note that experimental and theoretical information on small leaks, sodium-water interaction, and the subsequent distribution of hydrogen in a system, is scarce and of dubious validity.

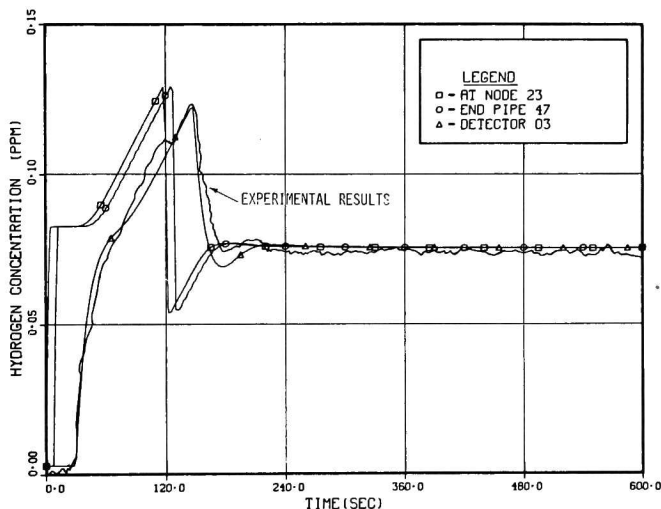


Fig. 29. Changes in Cover-gas Hydrogen Concentrations When Hydrogen-disengagement Half-life Is Reduced by a Factor of 1000

Most of the parameters governing hydrogen diffusion and transport throughout the system and its subsequent "evaporation" (or disengagement, if in bulk form) in the cover gas are not known. Some of the reaction parameters available, such as NaOH and HaH dissociation rates, are old data with large error limits obtained under laboratory conditions different from the actual operating conditions of the steam generator; and there is no quantitative information on how the reaction proceeds at the leak site. As a result, several assumptions had to be made and the results given in Sec. IX are dependent on these assumptions.

The contention is that the mathematical model is correct, since it is developed from basic principles. Values assumed for currently unknown parameters will be replaced with reliable experimental data, as they become available. In the meantime, the CCTL-DYSP will be used primarily to predict the response of the hydrogen and oxygen detectors during steam-generator leak-detection experiments in the CCTL.

Application of the CCTL-DYSP to a CRBRP steam-generator simulation will require some changes in the routines and additional input. For example, the program should account for (1) temperature variation from segment to segment (either to be calculated or supplied as input), (2) hydrogen diffusion through the steam-generator walls, and (3) other sources and sinks of hydrogen and oxygen that may be significant. These changes will not affect the program structure; rather they will add terms to the hydrogen and oxygen sources in the appropriate routine.

APPENDIX A

Mathematical Model Used in CCTL Dynamic
Simulation Program (CCTL-DYSP)

The equations and notations described in this appendix are identical to those used in CCTL-DYSP; algebraic operations are written mostly in FORTRAN symbolics.

1. An Ideal Mixing Plenum

In "ideal mixing" it is assumed the inlet stream of sodium into a segment is instantly and totally mixed with the sodium in the segment. The equations describing concentration changes of the four reaction products (i.e., C1 for NaH, C2 for NaOH, C3 for Na₂O, and C4 for hydrogen) are

$$DC1(I) = (W(I)*(C1(II) - C1(I)) + CC1)/M(I) + S1(I), \quad (A.1)$$

$$DC2(I) = (W(I)*(C2(II) - C2(I)) + CC2)/M(I) + S2(I), \quad (A.2)$$

$$DC3(I) = (W(I)*(C3(II) - C3(I)) + CC3)/M(I) + S3(I), \quad (A.3)$$

and

$$DC4(I) = (W(I)*(C4(II) - C4(I)) + CC4)/M(I) + S4(I), \quad (A.4)$$

where

DC1-DC4 = time derivatives of the appropriate reaction-product concentrations,

I = index of the variables or number of node for which concentrations are calculated,

II = index number of the segment from which the main flow enters the Ith segment (usually II = I - 1),

M(I) = mass of the Ith segment,

W(I) = total flow through the Ith segment,

and CC1-CC4 account for concentration changes other than those due to the main-stream inlet and outlet for the four reaction products.

For multiple entry nodes, the following equations apply:

For node 22,

$$CC1 = WEX*(C1(3) - C1(21)). \quad (A.5)$$

For node 27,

$$CC1 = WT1*Cl(50) + WT3*Cl(48) + WT4*Cl(46) - WDET*Cl(27), \quad (A.6)$$

where

$$WDET = WT1 + WT3 + WT4. \quad (A.7)$$

For node 29,

$$CC1 = WCT*(Cl(43) - Cl(28)). \quad (A.8)$$

The S terms in Eqs. A.1-A.4 are the reaction-product sources resulting from primary or secondary reactions and are given by

$$S1(I) = KK1*QS(I)/M(I) - DNAH, \quad (A.9)$$

$$S2(I) = KK2*QS(I)/M(I) - DNAOH, \quad (A.10)$$

$$S3(I) = KK3*QS(I)/M(I) + DNAOH, \quad (A.11)$$

and

$$S4(I) = KK4*QS(I)/M(I) + (DNAH + DNAOH)*0.5 - WH/M(I), \quad (A.12)$$

where

$QS(I)$ = leak rate at the Ith node,

WH = rate of hydrogen escape from the segment into the cover-gas plenum,

$$DNAH = RR1*Cl(I), \quad (A.13)$$

$$DNAOH = R3*Cl(I), \quad (A.14)$$

$RR1$ = NaH dissociation rate,

$$RR1 = 0.597*EXP(-3833/TK)*((PDIS - PH)/PDIS)^2 \quad (A.15)$$

TK = Kelvin temperature of sodium,

$$TK = (TEMP - 32)/1.8 + 273, \quad (A.16)$$

$TEMP$ = sodium temperature (in °F), which is an input value,

$PDIS$ = NaH dissociation pressure,

PH = hydrogen partial pressure,

and

R3 = NaOH dissociation rate, which is an input value.

Finally, the actual values of the reaction-product concentrations are obtained by integrating the derivatives in Eqs. A.1-A.4 by an integration routine. Presently a simple Euler formula is used, but any integration procedure can be chosen.

2. Node with Cover Gas

The term WH in Eq. A.12 is given by

$$WH = R1*(C4(I) - CHNA) \text{ for } CHNA > C4(I), \quad (A.17)$$

where

R1 = hydrogen-gas disengagement constant,

CHNA = hydrogen concentration in sodium that would be achieved under equilibrium conditions according to Sieverts' constant,

$$CHNA = KS*SQRT(PH), \quad (A.18)$$

and

KS = Sieverts' constant,

$$KS = EXP(1.9733 - 276.77/TK)*453.6/2.0116*10^{-6}. \quad (A.19)$$

The partial hydrogen pressure PH in the cover gas is calculated from the ideal gas laws, and is given by

$$DPH = (WHPU + WHCT)*554*TPLEN/VPLEN, \quad (A.20)$$

where

WHPU = hydrogen gas escaping through the pump,

WHCT = hydrogen gas escaping through the CCTL vessel,

TPLEN = absolute temperature in the cover gas,

TPLEN = TEMP + 460,

and

VPLEN = total volume of gas plenum, including the CCTL vessel, the expansion tank, and the pump tank.

Finally, DPH is integrated to obtain PH.

3. Pipe Node and Generating Delay Functions

A pipe in the system generates a time lag or holds up an event occurring at the pipe inlet for a period equivalent to the passage time through the pipe.

A time lag for a specified event is generated by storing the appropriate concentrations at the pipe-inlet node along with appropriate time values. Each pipe segment is allocated 100 memory locations. Pipe-inlet values are stored initially at constant time intervals. When the simulation starts, these values are stored whenever a change larger than PDEL in the pipe-inlet variable occurs; PDEL is usually 0.5 or 1%. When the outlet variable of a pipe segment is required, the lag time τ is first calculated by

$$\tau = M(I)/W(I). \quad (A.21)$$

Then the value of the variable is calculated by linear interpolation of the two closest variables available at time $t - \tau$ in a pipe function.

The secondary reactions in the pipe are accounted for by the following equations. Assuming FX1, FX2, FX3, and FX4 are the pipe-outlet variables at time $t - \tau$, the true pipe-outlet concentrations are given by

$$C1(I) = FX1 + S1(I)*\tau, \quad (A.22)$$

$$C2(I) = FX2 + S2(I)*\tau, \quad (A.23)$$

$$C3(I) = FX3 + S3(I)*\tau, \quad (A.24)$$

$$C4(I) = FX4 + S4(I)*\tau, \quad (A.25)$$

where

$$S1(I) = -RR1*FX1, \quad (A.26)$$

$$S2(I) = -R3*FX2, \quad (A.27)$$

$$S3(I) = -S2(I), \quad (A.28)$$

and

$$S4(I) = -(S1(I) + S2(I))*0.5. \quad (A.29)$$

4. Cold Trap

The cold trap causes reaction products to precipitate at a rate

$$W42 = BETA*(C1(42) - C1SAT), \quad (A.30)$$

and

$$W420 = \text{BETA} * (\text{C3}(42) - \text{C3SAT}), \quad (\text{A.31})$$

where

$W42$ = precipitation rate of NaH,

$W420$ = precipitation rate of Na_2O ,

BETA = dynamic cold-trap efficiency,

C1SAT = saturation concentration of NaH,

$$\text{C1SAT} = 453.6 * 10^{-6} / 23.9983 * \text{EXP}(13.93 - 6631.4 / \text{TCLT}), \quad (\text{A.32})$$

C3SAT = saturation concentration of Na_2O ,

$$\text{C3SAT} = 453.6 * 10^{-6} / 61.98 * \text{EXP}(16.131 - 6493.3 / \text{TCLT}), \quad (\text{A.33})$$

where

TCLT = absolute cold-trap temperature

$$\text{TCLT} = (\text{TCLT} - 32) / 1.8 + 273 \quad (\text{A.34})$$

5. Detectors

The derivative of a hydrogen-detector response is given by

$$\text{DPP} = (\text{CD1} + \text{CD4} - \text{CDET}(\text{N})) / \text{TDLE}(\text{N}), \quad (\text{A.35})$$

where

$\text{TDLE}(\text{N})$ = diffusion delay time of Nth hydrogen detector,

$\text{CDET}(\text{N})$ = response of Nth detector obtained by integrating DPP or the detector internal hydrogen concentration,

$$\text{CD1} = (\text{FX1} + \text{SD1} * \text{TAU}) * 1.0083 * 10^6 / 453.6, \quad (\text{A.36})$$

and

$$\text{CD4} = (\text{FX4} + \text{SD4} * \text{TAU}) * 2.0166 * 10^6 / 453.6. \quad (\text{A.37})$$

FX1 and FX4 are hydride and hydrogen concentrations, respectively, at the outside of detector membrane, and are equal to the monitored segment concentration at time $\text{TIME} - \text{TAU}$, where TAU is given by

$$\text{TAU} = \text{M}(\text{N1}) / \text{W}(\text{N1}) + \text{TLAG}(\text{N}). \quad (\text{A.38})$$

In Eq. A.38, $M(N1)$ and $W(N1)$ are the mass and the flow rate of the monitoring bypass pipe segment, and $TLAG$ is the time lag of the N th detector. The hydrogen-detector response in ppm is obtained by integrating Eq. A.35. The oxygen-detector response is calculated from

$$DPP = (CD3 - CDET(N))/TDLE(N), \quad (A.39)$$

where

$$CD3 = (FX3 + SD3*TAU)*16.0*10^6/453.6 \quad (A.40)$$

and

$$SD3 = R3*FX2. \quad (A.41)$$

The oxygen-meter response is obtained by integrating Eq. A.39. The readout of the hydrogen meter in the cover gas is proportional to the hydrogen partial pressure. The readout is converted to ppm by volume using the relation

$$CD4 = PH*10^6/(PH + PA), \quad (A.42)$$

where

PH = hydrogen partial pressure

and

PA = argon-cover-gas partial pressure.

The detector response is calculated by integrating

$$DPP = (CD4 - CDET(N))/TDLE(N), \quad (A.43)$$

where $CDET(N)$ is the detector response, and $TDLE(N)$ is the delay time of the N th detector.

APPENDIX B

Description of CCTL-DYSP

A simplified schematic of the simulation program is shown in Fig. B.1. The program is written in FORTRAN in a modular form. It has five calculating subroutines, a coordinating main program, two service subroutines for printing and plotting results, and a small integrating routine.

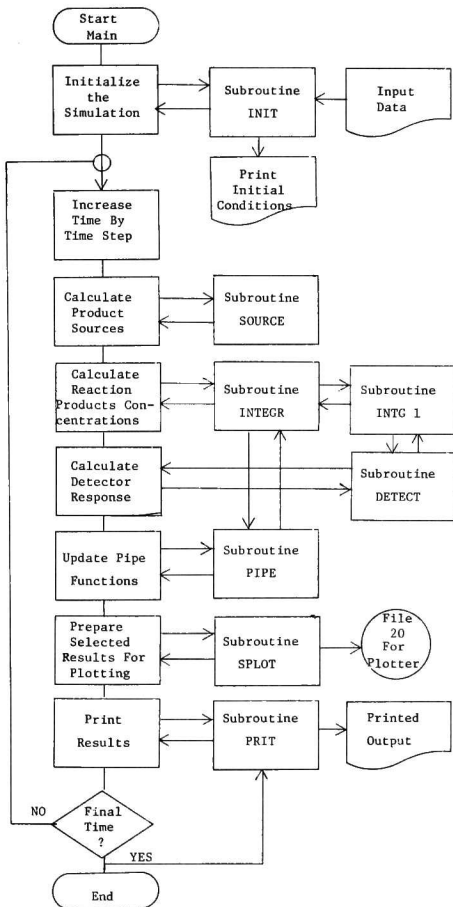


Fig. B.1. Simplified Schematic Flowchart of CCTL-DYSP

The main coordinating program first calls the INIT routine in which data are read in, initial values are calculated and printed, and the pipe initial function is set up. The program then proceeds to the dynamic phase by increasing time by a time step, and increasing the time-step counter by 1.

The first subroutine called in the dynamic section is SOURCE. This routine calculates the source of reaction products resulting from any type of chemical reaction at each loop segment. Equations A.5-A.19 are solved.

The second routine called is INTEGR, which computes the derivatives of all reaction-product concentrations in the loop segments and pipe outlets. This routine has access to the PIPE subroutine to compute pipe-outlet concentrations, and to the INTG1 routine, which performs the actual integration.

The main program then accesses the DETECT subroutine, which computes the appropriate detector responses.

After the variables for a time step have been calculated by appropriate integration of the differential equations, the program updates the inlet variables for the pipe segments by calling PIPE. The program then enters the PRIT routine, and, if requested, some data such as detector responses and concentrations at some of the nodes are printed.

Every TPR seconds--as determined by the input parameter--a complete "map" of the system is printed, which includes derivatives, sources, and actual concentration of the four reaction products at each segment and pipe outlet. The SPLOT routine is entered next, and user-selected data are stored in a specific file for later plotting.

Finally, the program checks the time; if it is less than the predetermined length of simulation, a time-step calculation is repeated. If the time is equal to the final simulation time, the program terminates by printing a final "map" of the system and print-plotting the results previously stored in a file. The listing of the program is given in Appendix C, and the input data are described in Appendix D.

APPENDIX C

Listing of CCTL-DYSP

CCTL.FORT

PRESENT DATE 8/11/76

DSK203

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5 C-----C
10 C
15 C CCTL-DYSP: A DYNAMIC SIMULATION PROGRAM TO CALCULATE HYDROGEN C
20 C AND OXYGEN CONCENTRATION IN WATER TO SODIUM LEAK EXPERIMENT IN C
25 C THE CORE COMPONENT TEST LOOP. C
30 C C
35 C PROGRAM CAPACITY: C
40 C 50 SEGMENTS C
45 C 7 DETECTORS C
50 C 4 REACTION PRODUCTS CONCENTRATIONS C
55 C 1 COMBINED COVER GAS PLENUM C
60 C 1 COLD TRAP C
65 C C
70 C-----C
75
80 C***** VOCABULARY *****C
85 C#####C
90 C#.....#C
95 C#.#C
100 C#.#C A - CROSS SECTION AREA OF SEGMENT (FT**2)
105 C#.#C ABSC - THE HEADING TO BE PRINTED ALONG THE ABCISAE OF
110 C#.#C GRAPHIC OUTPUT
115 C#.#C BETA - RATE AT WHICH NAH IS REMOVED IN THE COLD TRAP
120 C#.#C C1 - CONCENTRATION OF NAH (MOL/LB)
125 C#.#C C1SAT - SATURATION CONCENTRATION OF NAH AT COLD TRAP TEMPERATURES
130 C#.#C C2 - CONCENTRATION OF NAOH (MOL/LB)
135 C#.#C C3 - CONCENTRATION OF NA2O (MOL/LB)
140 C#.#C C4 - CONCENTRATION OF H2 (MOL/LB)
145 C#.#C CDET - DETECTOR READING IN PPM
150 C#.#C FIGTTL - TITLE GIVE TO A FIGURE DRAWN BY THE CALCOMP PLOTTER
155 C#.#C FINTIM - SIMULATION TIME FOR THIS RUN IN (SEC)
160 C#.#C IC - NODE NUMBERS FOR WHICH CONCENTRATIONS TO BE PLOTTED
165 C#.#C ICT - NODE NUMBERS FOR WHICH PPM CONC OF H2 IS PRINTED PER STEP
170 C#.#C IQ - NUMBER OF NODE AT WHICH LEAKAGE MIGHT OCCURE
175 C#.#C JPL - PLOTTING COUNTER
180 C#.#C JPR - PRINTING COUNTER
185 C#.#C JT - TIME STEP COUNTER
190 C#.#C K1 - FRACTION OF H2O LEAK TO: NA+H2O=NAOH+1/2H2(G)
195 C#.#C K2 - FRACTION OF H2O LEAK TO: 2NA+H2O=NAOH+NAH
200 C#.#C K3 - FRACTION OF H2O LEAK TO: 3NA +H2O=2NAH+NA2O
205 C#.#C K4 - FRACTION OF H2O LEAK TO: 2NA+H2O=NA2O+H2
206 C#.#C KH - IF 1 WATER LEAK, IF 2 HYDROGEN LEAK.
210 C#.#C L - LENGTH OF SEGMENT (FT)
215 C#.#C LG - SEGMENT IDENTIFICATION NUMBER: 0 NO SEGMENT
220 C#.#C 1 PLENUM MIXED SEGMENT
225 C#.#C 2 PIPE SEGMENT
230 C#.#C 3 PLENUM MIXING WITH COVER GA.
235 C#.#C 5 PLENUM WITH COVER AND MULTE.
240 C#.#C M - MASS OF SODIUM IN SEGMENT
245 C#.#C NAME - NAME OF APPROPRIATE VECTOR TO BE PLOTTED
250 C#.#C NGRAF - NO. OF CURVES TO BE PRINTED OR PLOTTED PER FIG.
255 C#.#C NNODE - NUMBER OF NODE TO WHICH DETECTOR IS CONNECTED
260 C#.#C NTYPE - TYPE OF DETECTOR USED MONITORING AT SEGMENT 'NODE'

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265 C#. NUDET - NUMBER OF DETECTORS IN THE SYSTEM .#C
270 C#. PA - ARGON PARTIAL PRESSURE IN COVER GAS .#C
275 C#. PDIS - NAH DISSOCIATION PRESSURE .#C
280 C#. PDEL - MAXIMUM PERMITTED CHANGE IN NODE 23 FOR PIPE UPDATA .#C
285 C#. PH - HYDROGEN PARTIAL PRESSURE IN COVER GAS (MM-HG) .#C
290 C#. PRT1 - IF TRUE INITIAL PIPE FUNCTION DISTRIBUTION WILL BE .#C
295 C#. PRINTED .#C
300 C#. PRT2 - RESERVED .#C
305 C#. PRT3 - RESERVED .#C
310 C#. PRT4 - RESERVED .#C
315 C#. PRT5 - IF TRUE A CALCUMP 580 PLOT OF THE PREDETERMINED VARI- .#C
320 C#. ABLES WILL BE PREPARED .#C
322 C#. PTDL - MAXIMUM PERMITTED TIME INTERVAL FOR PIPE UPDATE .#C
325 C#. Q - H2O LEAKAGE IN THE I-TH NODE (LBS/SEC) .#C
330 C#. R1 - RATE OF H2 DISENGAGEMENT FROM LIQUID NA TO COVER GAS (SEC-1) .#C
335 C#. R2 - RATE OF NAH DISSOCIATION  $NAH=NA+H$  (SEC-1*MM-HG-2) .#C
340 C#. R3 - RATE OF NAOH DISSOCIATION  $NAOH+NA=NA2O+H$  (SEC-1) .#C
345 C#. S1 - SOURCE OF NAH (MOL/SEC) .#C
350 C#. S2 - SOURCE OF NAOH (MOL/SEC) .#C
355 C#. S3 - SOURCE OF NA2O (MOL/SEC) .#C
360 C#. S4 - SOURCE OF H2 (MOL/SEC) .#C
365 C#. TQ - TIME AT WHICH LEAKAGE AT I-TH NODE STARTS (SEC) .#C
370 C#. TX - TIME AT WHICH LEAKAGE AT I-TH NODE TERMINATES (SEC) .#C
375 C#. TCLT - COLD TRAP TEMPERATURE (DEG F OR K) .#C
380 C#. TOLE - DIFFUSION TIME CONSTANT FOR DET. NICKEL MEMBRANE (SEC) .#C
385 C#. TEMP - SODIUM TEMPERATURE (DEG F) .#C
390 C#. TIME - CURENT SIMULATION TIME (SEC) .#C
395 C#. TLAG - TIME LAG BETWEEN DETECTOR SAMP.LINE INLET AND DETECTOR (SE.#C
400 C#. TMM - TOTAL SODIUM MASS IN CCTL (LBS) .#C
405 C#. TMT - TOTAL COOLANT TRANSIT TIME (SEC) .#C
410 C#. TPL - PLOTING INTERVAL (SEC) .#C
415 C#. TPR - PRINTING INTERVAL (SEC) .#C
420 C#. WCT - FLOW THROUGH THE COLD TRAP IN (GPM) .#C
425 C#. WS - TOTAL SODIUM FLOW IN CCTL (GPM) .#C
430 C#. WT1 - FLOW TO DETECTOR # 1 (LBS/SEC) .#C
435 C#. WT2 - FLOW TO DETECTOR # 2 (LBS/SEC) .#C
440 C#. WT3 - FLOW TO DETECTOR # 3 (LBS/SEC) .#C
445 C#. WT4 - FLOW TO DETECTOR # 4 (LBS/SEC) .#C
450 C#. .#C
455 C#####C
460
465 COMMON /BLK/ L,A,M,C1,C2,C3,C4,LG,WS,WCT,WT1,WT2,WT3,WT4,WEX,TEMP,
470 C FINTIM,RONA,DTMIN,DTMAX,S1,S2,S3,S4,JT,KS,TPR,IQ,ICT,W,JCT,
475 C WR,WA,WX,WB,WC,WQ,WE,Q,TQ,TX,QS,PDIS,PH,PA,K1,K2,K3,K4,R1,R2,R3,
480 C WHCT,WHPU,TPLEN,VPLEN,IC,TPL,CHNA,RR1,QX,QXT,QHT,C1SAT,BETA,
485 C ALFA,TMM,NPCT,NGRAF,NVECT,NAME,IPI,NUDET,NODE,NTYPE,
490 C TLAG,CDET,TOLE,C3SAT,PDEL,FIGTIL,PTDL,KH
495 COMMON /LUG/ TITLE,PRT1,PRT2,PRT3,PRT4,PRT5
500 COMMON /DUB/ TIME,DELT,DC1,DC2,DC3,DC4,ABSC
505 REAL*4 L(50),A(50),M(50),C1(50),C2(50),C3(50),C4(50),W(50)
510 REAL*4 S1(50),S2(50),S3(50),S4(50),Q(8),TQ(8),TX(8),QS(50)
515 REAL*4 K1,K2,K3,K4,KS,TITLE(18),TLAG(7),CDET(7),TOLE(7)
520 REAL*8 DC1(50),DC2(50),DC3(50),DC4(50),TIME,DELT,ABSC(4,10)

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525     LOGICAL PRT1,PRT2,PRT3,PRT4,PRT5
530     DIMENSION LG(50),IQ(8),IC(8),ICT(8),NGRAF(10),NVECT(10,5),
535     C NAME(10,15),IPI(50),NODE(7),NTYPE(7),FIGTTL(15,10)
540
545     CALL INIT
550     LV=1
555     QXT=0.
560     C4OLD=C4(23)
565     TOLD=0.
570     GOTO 20
575 C**** START TIME DEPENDENT CALCULATIONS
580   10  TIME=TIME+DELT
585     JT=JT+1
590     CALL SOURCE
595     CALL INTEGR
600     CALL DETECT
605 C**** UPDATE PIPE FUNCTIONS IF CHANGE > PDEL OR ELAPSED TIME MORE THEN .
610 C**** 0.5 SECONDS
615     TIM=TIME
620     CHNG=(C4OLD-C4(23))/C4OLD
625     CHTM=TIM-TOLD
630     IF(ABS(CHNG).LT.PDEL.AND.CHTM.LT.PTDL) GOTO 20
635     TOLD=TIM
640     C4OLD=C4(23)
645     DEL=DELT
650     CALL PIPE(TIM,DEL,0.0,1,C1(1),C2(1),C3(1),C4(1))
655     CALL PIPE(TIM,DEL,0.0,2,C1(3),C2(3),C3(3),C4(3))
660     CALL PIPE(TIM,DEL,0.0,3,C1(23),C2(23),C3(23),C4(23))
665     CALL PIPE(TIM,DEL,0.0,4,C1(27),C2(27),C3(27),C4(27))
670     CALL PIPE(TIM,DEL,0.0,5,C1(29),C2(29),C3(29),C4(29))
675     CALL PIPE(TIM,DEL,0.0,6,C1(6),C2(6),C3(6),C4(6))
680     CALL PIPE(TIM,DEL,0.0,7,C1(25),C2(25),C3(25),C4(25))
685     CALL PIPE(TIM,DEL,0.0,8,C1(42),C2(42),C3(42),C4(42))
690     CALL PIPE(TIM,DEL,0.0,10,RR1,PH,CHNA,0.0)
695 C**** PERFORM TOTAL HYDROGEN BALANCE CALCULATIONS FOR THIS TIME STEP
700   20  QX=0.
705     QHT=0.
710     DO 92 I=1,50
715     IF(LG(I).EQ.0) GOTO 92
720     QHT=QHT+(0.5*C1(I)+0.5*C2(I)+C4(I))*M(I)
725     QX=QX+QS(I)
730   92  CONTINUE
735     QXT=QXT+QX*DELT
740     QHT=QHT+PH*VPLEN/(IPLEN*554.0)
745     ALFA=(0.5*C1(ICT(1))+C4(ICT(1)))*TMM/QHT
750     CALL SPLOT(LV)
755     CALL PRIT(LV)
760     TIM=TIME
765     LV=2
770     IF(FINTIM-TIM.GT.DELT/2) GOTO 10
775     CALL PRIT(3)
780     CALL SPLOT(3)
785     STOP

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790      END
795
800 C -----C
805 C
810 C      SUBROUTINE INIT
815 C      THIS SUBROUTINE INITIALIZES THE PROGRAM, READS INPUT DATA
820 C      AND SUPPLIES DEFAULT VALUES TO DATA NOT IN INPUT STREAM
825 C
830 C -----C
835
840      SUBROUTINE INIT
845      COMMON /BLK/ L,A,M,C1,C2,C3,C4,LG,WS,WCT,WT1,WT2,WT3,WT4,WEX,TEMP,
850      C FINTIM,RONA,DTMIN,DTMAX,S1,S2,S3,S4,JT,KS,TPR,IQ,ICT,W,JCT,
855      C WR,WA,WX,WB,WC,WD,WE,Q,TQ,TX,QS,PDIS,PH,PA,K1,K2,K3,K4,R1,R2,R3,
860      C WHCT,WHPU,TPLEN,VPLEN,IC,TPL,CHNA,RR1,QX,QXT,QHT,C1SAT,BETA,
865      C ALFA,TMM,NPICT,NGRAF,NVECT,NAME,IPI,NUDET,NODE,NTYPE,
870      C TLAG,CDET,TDLE,C3SAT,PDEL,FIGTTL,PTDL,KH
875      COMMON /LOG/ TITLE,PRT1,PRT2,PRT3,PRT4,PRT5
880      COMMON /DUB/ TIME,DELTA,DC1,DC2,DC3,DC4,ABSC
885      REAL*4 L(50),A(50),M(50),C1(50),C2(50),C3(50),C4(50),W(50)
890      REAL*4 S1(50),S2(50),S3(50),S4(50),Q(8),TQ(8),TX(8),QS(50)
895      REAL*4 K1,K2,K3,K4,KS,TITLE(18),TLAG(7),CDET(7),TDLE(7)
900      REAL*8 DC1(50),DC2(50),DC3(50),DC4(50),TIME,DELTA,ABSC(4,10)
905      LOGICAL PRT1,PRT2,PRT3,PRT4,PRT5
910      REAL*4 MOL
915      DIMENSION LG(50),IQ(8),IC(8),ICT(8),NGRAF(10),NVECT(10,5),
920      C NAME(10,15),IPI(50),NODE(7),NTYPE(7),FIGTTL(15,10)
925      DIMENSION ADAT(20)
930      DATA PI/3.1416/,CFPG/.13368981/,ADA/'9999'/
935 C
940      1 READ 180,ADAT
945      PRINT 190,ADAT
950      IF (ADAT(1).NE.ADA) GOTO 1
955      REWIND 5
960      NAMELIST /INLST/ L,LG,A,C1,C2,C3,C4,Q,TQ,TX,IQ,IC,ICT
965      C /PARAM/ TEMP,WS,WCT,WT1,WT2,PH,PA,K1,K2,K3,K4,R1,R3,BETA,C1SAT,
970      C WT3,WT4,WEX,FINTIM,DELTA,DTMIN,DTMAX,TPR,VPLEN,TPL,JCT,
975      C PRT1,PRT2,PRT3,PRT4,PRT5,BETA,TCLT,PDEL,PTDL,KH
980      C /DTCTR/ NUDET,NODE,NTYPE,TDLE,TLAG
985      READ 200,TITLE
990      READ (5,INLST)
995      READ (5,PARAM)
1000      READ (5,DTCTR)
1005      READ 210
1010      READ 170,NPICT
1015      READ 170,NGRAF
1020      DO 3 N=1,NPICT
1025      NN=NGRAF(N)
1030      READ 170,(NVECT(N,I),I=1,NN)
1035      READ 220,((NAME(N,(I-1)*3+J),J=1,3),I=1,NN)
1040      READ 230,(ABSC(I,N),I=1,4)
1045      READ 200,(FIGTTL(I,N),I=1,15)
1050      3 CONTINUE

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1055      RONA=59.566-TEMP*(7.9504E-3+TEMP*(2.872E-7-TEMP*6.035E-11))
1060      MOL=453.6/18.02
1065      QX=0.
1070      QXT=0.
1075      WS=WS*CFPG*RONA/60.
1080      WCT=WCT*CFPG*RONA/60.
1085      WT1=WT1*CFPG*RONA/60.
1090      WT2=WT2*CFPG*RONA/60.
1095      WT3=WT3*CFPG*RONA/60.
1100      WT4=WT4*CFPG*RONA/60.
1105      WEX=WEX*CFPG*RONA/60.
1110      WA=WS-WEX
1115      WX=WA-WT1-WT2
1120      WB=WX+WEX
1125      WC=WB-WT3
1130      WD=WC-WT4-WCT
1135      WE=WD+WT1+WT2+WT3+WT4
1140      WR=WE+WCT
1145      TMM=0.
1150      DU 5 I=1,8
1155      5 Q(I)=Q(I)*MOL
1160      C1(I)=C1(I)*453.6/23.9986
1165      C2(I)=C2(I)*453.6/39.9983
1170      C3(I)=C3(I)*453.6/61.98
1175      C4(I)=C4(I)*453.6/2.0166
1180      TCLT=(TCLT-32.0)/1.8+273.0
1185      C1SAT=453.6E-6/23.9983*EXP(13.97-6631.4/TCLT)
1190      C3SAT=453.6E-6/61.98*EXP(16.131-6493.3/TCLT)
1195      IF(C1(I).EQ.0.0) C1(I)=C1SAT
1200      IF(C3(I).EQ.0.0) C3(I)=C3SAT
1205      DU 10 I=1,50
1210      IPI(I)=0
1215      C1(I)=C1(I)
1220      C2(I)=C2(I)
1225      C3(I)=C3(I)
1230      C4(I)=C4(I)
1235      IF(LG(I).NE.0) GOTU 9
1240      C3(I)=0.
1245      C4(I)=0.
1250      C1(I)=0.
1255      C2(I)=0.
1260      9 W(I)=0.
1265      S1(I)=0.
1270      S2(I)=0.
1275      S3(I)=0.
1280      S4(I)=0.
1285      QS(I)=0.
1290      M(I)=L(I)*A(I)*RUNA
1295      TMM=TMM+M(I)
1300      DC1(I)=0.
1305      DC2(I)=0.
1310      DC3(I)=0.
1315      DC4(I)=0.

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1320      10 CONTINUE
1325 C**** INITIALIZE DETECTOR READING
1330      DO 11 N=1,NUDET
1335          NTP=NTYPE(N)
1340          GOTO (12,13,14), NTP
1345      12 CDET(N)=(0.5*C1(1)+C4(1))*2.0166E+6/453.3
1350          GOTO 11
1355      13 CDET(N)=C3(1)*16.0E+6/453.3
1360          GOTO 11
1365      14 CDET(N)=PH*1.0E+6/(PA+PH)
1370      11 CONTINUE
1375          M(46)=M(46)+M(45)
1380          M(48)=M(48)+M(47)
1385          M(50)=M(50)+M(49)
1390          TM=0.
1395          DO 15 I=1,30
1400      15 TM=TM+M(I)
1405          TM=TM-M(6)
1410          TMT=TM/WS
1415          IP=0
1420          CALL PIPE(TIME,DELT,0.,IP,C1(1),C2(1),C3(1),C4(1))
1425          TK=(TEMP-32.)/1.8+273.
1430          TPLEN=TEMP+460.
1435          KS=EXP(1.9733-276.77/TK)*453.6/2.0116*1.E-6
1440          PDIS=EXP(26.71-14046.0/TK)
1445          R2=0.597*EXP(-3833/TK)
1450 C
1455 C**** CALCULATE TOTAL FLOW THROUGH EACH SEGMENT
1460          W(1)=WR
1465          W(2)=WS
1470          W(3)=WS
1475          W(4)=WA
1480          W(5)=WA
1485          W(6)=WT1+WT2
1490          W(7)=WA
1495          DO 20 I=8,21
1500      20 W(I)=WX
1505          W(22)=WB
1510          W(23)=WB
1515          W(24)=WC
1520          W(25)=WC
1525          W(26)=WD
1530          W(27)=WE
1535          W(28)=WE
1540          W(29)=WR
1545          W(30)=WR
1550          W(41)=WCT
1555          W(42)=WCT
1560          W(43)=WCT
1565          W(45)=WT4
1570          W(46)=WT4
1575          W(47)=WT3
1580          W(48)=WT3

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1585      W(49)=WT1
1590      W(50)=WT1
1595 C**** SET APPROPRIATE PIPE FUNCTION NUMBERS TO PIPE SEGMENTS
1600      IPI(2)=1
1605      IPI(4)=2
1610      IPI(24)=3
1615      IPI(47)=3
1620      IPI(48)=3
1625      IPI(28)=4
1630      IPI(30)=5
1635      IPI(41)=7
1640      IPI(45)=7
1645      IPI(46)=7
1650      IPI(49)=6
1655      IPI(50)=6
1660      IPI(43)=8
1665      BETA=BETA*W(42)/M(42)
1670      CALL SOURCE
1675      CALL PIPE(TIME,DELT,0.0,10,RR1,PH,CHNA,0.0)
1680 C
1685 C**** PRINT INITIAL DATA
1690      PRINT 300,TITLE
1695      PRINT 100
1700      PRINT 110, IQ,Q,TQ,TX
1705      YK1=K2+2.*K3
1710      YK2=K1+K2
1715      YK3=K3+K4
1720      YK4=0.5*K1+K4
1725      PRINT 150,K1,K2,K3,K4,YK1,YK2,YK3,YK4
1730      PRINT 120, POIS
1735      PRINT 130, TEMP,TK,RONA,TMM,VPLEN,BETA,C1SAT,C3SAT,TMT,TCLT,KS
1740      PRINT 140, WS,WCT,WT1,WT2,WT3,WT4,WEX,WA,WX,WB,WC,WD,WE,WR
1745      PRINT 160,(N,NTYPE(N),NODE(N),TLAG(N),TDLE(N),N=1,NUDET)
1750      99 RETURN
1755      100 FORMAT(1H,' LEAKAGE DATA FOR THIS CASE ARE:')
1760      110 FORMAT(1H0,'FOR NODE SEGMENT #',8I12/)
1765      C ' THE LEAKAGE IN MOL/SEC IS',8E12.4/
1770      C ' THE LEAK STARTS AT TIME -',8F12.2/
1775      C ' THE LEAK IS TERMINATED AT',8F12.2/)
1780      120 FORMAT('0THE NAH DISSOCIATION PRESSURE IN MM-HG IS',F12.3)
1785      130 FORMAT(' SODIUM TEMPERATURE IN (DEG-F) IS',F12.2/
1790      C ' SODIUM TEMPERATURE IN (DEG-K) IS',F12.2/
1795      C ' SODIUM DENSITY IN (LBS/CUF) IS',F12.2/
1800      C ' TOTAL WEIGHT OF SODIUM IN THE SYSTEM (LB)',F12.2/
1805      C ' COVER GAS PLENUM VOLUME (CUF)',F12.2/
1810      C ' COLD TRAP DYNAMIC EFFICIENCY (1/SEC) IS',E12.4/
1815      C ' NAH SATURATION CONC. AT COLD TRAP(MOL/LB)',E12.4/
1820      C ' NA2O SATURATION CNC. AT COLD TRAP(MOL/LB)',E12.4/
1825      C ' TOTAL TRANSIT TIME IN CCTL (SEC) IS',F12.2/
1830      C ' COLD TRAP TEMPERATURE IN (DEG-K) IS',F12.2/
1835      C ' SIEVERTS CONSTANT IN (MOL/(LB*TORR**-2))',E12.4)
1840      140 FORMAT('0TOTAL SODIUM FLOW IN (LBS/SEC) IS',F12.4,
1845      C/30X,'WCT',9X,F12.4/30X,'WT1',9X,F12.4/30X,'WT2',9X,F12.4/

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1850      C 30X,'WT3',9X,F12.4/30X,'WT4',9X,F12.4/30X,'WEX',9X,F12.4/
1855      C 30X,'WA ',9X,F12.4/30X,'WX ',9X,F12.4/30X,'WB ',9X,F12.4/
1860      C 30X,'WC ',9X,F12.4/30X,'WD ',9X,F12.4/30X,'WE ',9X,F12.4/
1865      C 30X,'WR ',9X,F12.4//)
1870      170 FORMAT(10(I2,1X))
1875      150 FORMAT(1X,F4.2,' OF THE LEAK GOES TO  NA+H2O=NAOH+1/2H2(G)'/
1880      C      1X,F4.2,' OF THE LEAK GOES TO  2NA+H2O=NAOH+NAH'/
1885      C      1X,F4.2,' OF THE LEAK GOES TO  4NA+H2O=2NAH+NA2O'/
1890      C      1X,F4.2,' OF THE LEAK GOES TO  2NA+H2O=NA2O+H2'/
1895      C      1X,F4.2,' MOL OF THE LEAK IS TRANSFORMED TO NAH'/
1900      C      1X,F4.2,' MOL OF THE LEAK IS TRANSFORMED TO NAOH'/
1905      C      1X,F4.2,' MOL OF THE LEAK IS TRANSFORMED TO NA2O'/
1910      C      1X,F4.2,' MOL OF THE LEAK IS TRANSFORMED TO H2(G)')
1915      160 FORMAT(1H0,' DETECTOR NO ',I1,' OF TYPE ',I1,' IS CONECTED',
1920      C      C ' TO NODE ',I2,' HAS A LAG OF ',F5.2,'SEC AND A DELAY OF',
1925      C      C F5.2,'SEC')
1930      180 FORMAT(20A4)
1935      190 FORMAT(10X,20A4)
1940      200 FORMAT(18A4)
1945      210 FORMAT(80X)
1950      220 FORMAT(5(3A4,1X))
1955      230 FORMAT(4A8)
1960      300 FORMAT('1',20('1'),18A4,20('1'))//)
1965      END
1970
1975 C-----C
1980 C
1985 C      SUBROUTINE SOURCE.
1990 C      IN THIS SUBROUTINE SOURCES AND SINKS OF THE REACTION PRODUCTS
1995 C      ARE CALCULATED
2000 C
2005 C-----C
2010
2015      SUBROUTINE SOURCE
2020      COMMON /BLK/ L,A,M,C1,C2,C3,C4,LG,WS,WCT,WT1,WT2,WT3,WT4,WEX,TEMP,
2025      C      FINTIM,RUNA,DTMIN,DTMAX,S1,S2,S3,S4,JT,KS,TPR,IQ,ICT,W,JCT,
2030      C      WR,WA,WX,WB,WC,WD,WE,Q,TQ,TX,QS,PDIS,PH,PA,K1,K2,K3,K4,R1,R2,R3,
2035      C      WHCT,WHPU,TPLEN,VPLEN,IC,TPL,CHNA,RR1,UX,QXT,QHT,C1SAT,BETA,
2040      C      ALFA,TMM,NPICT,NGRAF,NVECT,NAME,IPI,NUDET,NODE,NTYPE,
2045      C      TLAG,CDET,TDLE,C3SAT,PDEL,FIGTTL,PTDL,KH
2050      COMMON /LOG/ TITLE,PRT1,PRT2,PRT3,PRT4,PRT5
2055      COMMON /DUB/ TIME,DELT,DC1,DC2,DC3,DC4,ABSC
2060      REAL*4 L(50),A(50),M(50),C1(50),C2(50),C3(50),C4(50),W(50)
2065      REAL*4 S1(50),S2(50),S3(50),S4(50),Q(8),TQ(8),TX(8),QS(50)
2070      REAL*4 K1,K2,K3,K4,KS,TITLE(18),TLAG(7),CDET(7),TDLE(7)
2075      DIMENSION LG(50),IQ(8),IC(8),ICT(8),NGRAF(10),NVECT(10,5),
2080      C      NAME(10,15),IPI(50),NODE(7),NTYPE(7),FIGTTL(15,10)
2085      REAL*4 KK1,KK2,KK3,KK4
2090      REAL*8 DC1(50),DC2(50),DC3(50),DC4(50),TIME,DELT,ABSC(4,10)
2095      LOGICAL PRT1,PRT2,PRT3,PRT4,PRT5
2100 C
2105 C**** CALCULATE REACTION RATES
2110      GOTO (1,3),KH

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2110      1 KK1=K2+2*K3
2115      KK2=K1+K2
2120      KK3=K3+K4
2125      KK4=0.5*K1+K4
2126      GOTO 4
2127      3 KK1=2*K1
2128      KK2=0
2129      KK3=0
2130      KK4=1.-K1
2134      4 RR1=((PDIS-PH)/PDIS)*ABS((PDIS-PH)/PDIS)*R2
2135      CHNA=KS*SQR1(PH)
2140 C
2145 C**** DETERMINE LEAKAGE SOURCES
2150      DO 2 I=1,8
2155      I2=IQ(I)
2160      QS(I2)=0.0
2165      IF (TIME*GE.TQ(I).AND.TIME.LE.TX(I)) QS(I2)=Q(I)
2170      2 CONTINUE
2175 C
2180 C**** CALCULATE SOURCES IN MOL/SEC
2185      DO 10 I=1,50
2190      IF (LG(I).EQ.0.OR.LG(I).EQ.2) GOTO 10
2195      DNAH=RR1*C1(I)
2200      DNAOH=R3*C2(I)
2205      11 S1(I)=KK1*QS(I)/M(I)-DNAH
2210      S2(I)=KK2*QS(I)/M(I)-DNAOH
2215      S3(I)=KK3*QS(I)/M(I)+DNAOH
2220      S4(I)=KK4*QS(I)/M(I)+(DNAH+DNAOH)*0.5
2225      10 CONTINUE
2230 C**** ACCOUNT FOR POSSIBLE BUBBLE MIGRATION IN THE CCTL VESSEL
2235      W25=0.
2240      W26=0.
2245      WHCT=0.
2250      WHPU=0.
2255      IF (C4(25).LE.C4(26)) GOTO 21
2260      W25=R1*(C4(25)-C4(26))*M(25)
2265      21 IF (C4(26).LE.C4(27)) GOTO 22
2270      W26=R1*(C4(26)-C4(27))*M(26)
2275      22 C27=0.5*(C4(27)+C4(26)+0.5*(C1(27)+C1(26)))
2280      IF (C27.LE.CHNA) GOTO 23
2285      WHCT=R1*(C27-CHNA)*M(27)
2290      23 C01=0.5*(C4(1)+C4(30)+0.5*(C1(1)+C1(30)))
2295      IF (C01.LE.CHNA) GOTO 24
2300      WHPU=R1*(C01-CHNA)*M(1)
2305 C**** ACCOUNT FOR COLD TRAP NAH REMOOVAL
2310      24 W42=0.0
2315      W420=0.0
2320      IF (LG(42).EQ.0) GOTO 25
2325      W42=BETA*(C1(42)-C1SAT)
2330      W420=BETA*(C3(42)-C3SAT)
2335      IF (W42.LT.0.0) W42=0.0
2340      IF (W420.LT.0.0) W420=0.0
2345      25 S4(25)=S4(25)-W25/M(25)

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2350      S4(26)=S4(26)+(W25-W26)/M(26)
2355      S4(27)=S4(27)+(W26-WHCT)/M(27)
2360      S4(1)=S4(1)-WHPU/M(1)
2365      S1(42)=S1(42)-W42
2370      S3(42)=S3(42)-W42D
2375      RETURN
2380      END
2385
2390 C -----C
2395 C
2400 C      SUBROUTINE INTEGR.
2405 C      IN THIS ROUTINE CONCENTRATION OF THE VARIOUS REACTION PRODUCTS
2410 C      FOR EACH SEGMENT ARE CALCULATED.
2415 C
2420 C -----C
2425
2430      SUBROUTINE INTEGR
2435      COMMON /BLK/ L,A,M,C1,C2,C3,C4,LG,WS,WCT,WT1,WT2,WT3,WT4,WEX,TEMP,
2440      C FINTIM,RONA,DTMIN,DTMAX,S1,S2,S3,S4,JT,KS,TPR,IQ,ICT,W,JCT,
2445      C WR,WA,WX,WB,WC,WD,WE,Q,TQ,TX,QS,PDIS,PH,PA,K1,K2,K3,K4,R1,R2,R3,
2450      C WHCT,WHPU,TPLEN,VPLEN,IC,TPL,CHNA,RR1,QX,QXT,QHT,C1SAT,BETA,
2455      C ALFA,TMM,NPCT,NGRAF,NVECT,NAME,IPI,NUDET,NODE,NTYPE,
2460      C TLAG,CDET,TDLE,C3SAT,PDEL,FIGTTL,PTDL,KH
2465      COMMON /LOG/ TITLE,PRT1,PRT2,PRT3,PRT4,PRT5
2470      COMMON /DUB/ TIME,DELT,DC1,DC2,DC3,DC4,ABSC
2475      REAL*4 L(50),A(50),M(50),C1(50),C2(50),C3(50),C4(50),W(50)
2480      REAL*4 S1(50),S2(50),S3(50),S4(50),Q(8),TQ(8),TX(8),QS(50)
2485      REAL*4 K1,K2,K3,K4,KS,TITLE(18),TLAG(7),CDET(7),TDLE(7)
2490      REAL*8 DC1(50),DC2(50),DC3(50),DC4(50),TIME,DELT,ABSC(4,10)
2495      LOGICAL PRT1,PRT2,PRT3,PRT4,PRT5
2500      DIMENSION LG(50),IQ(8),IC(8),ICT(8),NGRAF(10),NVECT(10,5),
2505      C NAME(10,15),IPI(50),NODE(7),NTYPE(7),FIGTTL(15,10)
2510 C
2515 C**** CALCULATE DERIVATIVES FOR VARIABLES TO BE INTEGRATED AND S*TAU
2520 C**** VALUES FOR PIPE SEGMENTS
2525      DO 10 I=1,50
2530      IF(LG(I).EQ.0) GOTO 10
2535      CC1=0.
2540      CC2=0.
2545      CC3=0.
2550      CC4=0.
2555      LLG=LG(I)
2560 C**** CALCULATE DERIVATIVES FOR MIXING PLENUM NODES
2565      5 II=-1
2570      IF(I.EQ.1)II=30
2575      IF(I.EQ.6)II=7
2580      IF(I.EQ.7)II=5
2585      GOTO (4,10,4,8,8),LLG
2590      4 DC1(I)=(W(I)*(C1(II)-C1(I)))+(CC1)/M(I)+S1(I)
2595      DC2(I)=(W(I)*(C2(II)-C2(I)))+(CC2)/M(I)+S2(I)
2600      DC3(I)=(W(I)*(C3(II)-C3(I)))+(CC3)/M(I)+S3(I)
2605      DC4(I)=(W(I)*(C4(II)-C4(I)))+(CC4)/M(I)+S4(I)
2610      GOTO 10

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2615 C**** MULTIPLE ENTRY NODES
2620   8 IF(I,NE,22) GOTO 7
2625   CC1=WEX*(C1(3)-C1(21))
2630   CC2=WEX*(C2(3)-C2(21))
2635   CC3=WEX*(C3(3)-C3(21))
2640   CC4=WEX*(C4(3)-C4(21))
2645   GOTO 4
2650   7 IF(I,NE,27) GOTO 2
2655   WDET=WT1+WT2+WT3+WT4
2660   CC1=WT1*C1(50)+WT2*C1(48)+WT3*C1(48)+WT4*C1(46)-WDET*C1(27)
2665   CC2=WT1*C2(50)+WT2*C2(48)+WT3*C2(48)+WT4*C2(46)-WDET*C2(27)
2670   CC3=WT1*C3(50)+WT2*C3(48)+WT3*C3(48)+WT4*C3(46)-WDET*C3(27)
2675   CC4=WT1*C4(50)+WT2*C4(48)+WT3*C4(48)+WT4*C4(46)-WDET*C4(27)
2680   GOTO 4
2685   2 IF(I,NE,29) GOTO 1
2690   CC1=WCT*(C1(43)-C1(28))
2695   CC2=WCT*(C2(43)-C2(28))
2700   CC3=WCT*(C3(43)-C3(28))
2705   CC4=WCT*(C4(43)-C4(28))
2710   GOTO 4
2715 C**** WRONG SEGMENT IDENTIFICATION NUMBER IF PROGRAM ENTERS THIS SECTION
2720   1 PRINT 100,I
2725   10 CONTINUE
2730   DPH=(WHPU+WHCI)*554.0*TPLEN/VPLEN
2735 C**** CALCULATE CONCENTRATION IN SEGMENTS BY INTEGRATION
2740   IP=0
2745   DO 20 I=1,50
2750   LLG=LG(I)
2755   IF(LLG,EQ,0) GOTO 20
2760   IF(LLG,EQ,2) GOTO 21
2765   CALL INTG1(I,C1(I),DC1(I),DELT)
2770   CALL INTG1(I,C2(I),DC2(I),DELT)
2775   CALL INTG1(I,C3(I),DC3(I),DELT)
2780   CALL INTG1(I,C4(I),DC4(I),DELT)
2785   GOTO 20
2790   21 TAU=M(I)/W(I)
2795   TIM=TIME
2800   DEL=DELT
2805   IF(TAU.GT.TIME) TAU=TIME
2810   IP=IPI(I)
2815   CALL PIPE(TIM,DEL,TAU,IP,FX1,FX2,FX3,FX4)
2820   CALL PIPE(TIM,DEL,TAU,10,X1,X2,X3,X4)
2825   S1(I)=-((X1+RR1)/2.*FX1
2830   S2(I)=-R3*FX2
2835   S3(I)=-S2(I)
2840   S4(I)=-((S1(I)+S2(I))*0.5
2845   C1(I)=FX1+S1(I)*TAU
2850   C2(I)=FX2+S2(I)*TAU
2855   C3(I)=FX3+S3(I)*TAU
2860   C4(I)=FX4+S4(I)*TAU
2865   IF(C1(I).LE,0.0) C1(I)=0.0
2870   IF(C2(I).LE,0.0) C2(I)=0.0
2875   IF(C3(I).LE,0.0) C3(I)=0.0

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2880      IF(C4(I).LE.0.0) C4(I)=0.0
2885      20 CONTINUE
2890      CALL INTG1(1,PH,DPH,DELT)
2895      RETURN
2900      100 FORMAT(1H1,///1H,20(' '), ' ERROR IN SEGMENT IDENTIFICATION NUMBER
2905      C, CHECK LG('I2,') ',20(' '*'))
2910      END
2915
2920 C-----C
2925 C
2930 C      SUBROUTINE INTG.
2935 C      IN THIS SUBROUTINE THE DERIVATIVES OF THE SYSTEM
2940 C      VARIABLES WILL BE INTEGRATED USING EULER INTEGRATION METHOD
2945 C      PARAMETERS:
2950 C          I - INDEX (FOR FUTURE USE)
2955 C          Y - VARIABLE VALUE TO BE INTEGRATED
2960 C          DY - DERIVATIVE OF VARIABLE
2965 C          DT - DELT - TIME INCREMENT
2970 C
2975 C-----C
2980
2985      SUBROUTINE INTG1(I,Y,DY,DT)
2990 C
2995      Y=Y+DY*DT
3000      RETURN
3005      END
3010
3015 C-----C
3020 C
3025 C      SUBROUTINE PRIT.
3030 C      IN THIS SUBROUTINE THE RESULTS ARE BEING PRINTED
3035 C      PARAMETER IPZ =
3040 C          1 PRINT INITIAL CONDITIONS
3045 C          2 PRINT A LINE OF SELECTED RESULTS EVERY
3050 C             JTP TIME STEPS
3055 C          3 PRINT FINAL MAP
3060 C
3065 C-----C
3070
3075      SUBROUTINE PRIT(IPZ)
3080 C**** THIS ROUTINE WILL PRINT CONCENTRATION AT ALL SEGMENTS AT TIME T.
3085      COMMON /BLK/ L,A,M,C1,C2,C3,C4,LG,WS,WCT,WT1,WT2,WT3,WT4,WEX,TEMP,
3090      C FINTIM,RUNA,DTMIN,DTMAX,S1,S2,S3,S4,JT,KS,TPR,IQ,ICT,W,JCT,
3095      C WR,WA,WX,WB,WC,WD,WE,Q,TQ,TX,QS,PDIS,PH,PA,K1,K2,K3,K4,R1,R2,R3,
3100      C WHCT,WHPU,TLEN,VLEN,IC,TPL,CHNA,RR1,QX,QXT,QHT,C1SAT,BETA,
3105      C ALFA,TMM,NPCT,NGRAF,NVECT,NAME,IP1,NUDET,NODE,NTYPE,
3110      C TLAG,CDET,TDLE,C3SAT,PDEL,FIGTTL,PTDL,KH
3115      COMMON /LOG/ TITLE,PR11,PR12,PR13,PR14,PR15
3120      COMMON /DUB/ TIME,DELT,DC1,DC2,DC3,DC4,ABSC
3125      REAL*4 L(50),A(50),M(50),C1(50),C2(50),C3(50),C4(50),W(50)
3130      REAL*4 S1(50),S2(50),S3(50),S4(50),Q(8),TQ(8),TX(8),QS(50)
3135      REAL*4 K1,K2,K3,K4,KS,TITLE(18),TLAG(7),CDET(7),TDLE(7)
3140      REAL*8 DC1(50),DC2(50),DC3(50),DC4(50),TIME,DELT,ABSC(4,10)

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3145 LOGICAL PRT1,PRT2,PRT3,PRT4,PRT5
3150 DIMENSION LG(50),IQ(8),IC(8),ICT(8),NGRAF(10),NVECT(10,5),
3155 C NAME(10,15),IPI(50),NODE(7),NTYPE(7),FIGTTL(15,10)
3160 DIMENSION CHX(10)
3165 DATA JPR,JTP,JTI/1,0,0/
3170 TIM=TIME
3175 GOTO (10,20,30), IPZ
3180 10 PRINT 300,TITLE
3185 PRINT 130
3190 PRINT 140, (I,LG(I),L(I),A(I),M(I),W(I),QS(I),I=1,50)
3195 PRINT 300,TITLE
3200 PRINT 100
3205 22 PRINT 110 , TIME,JT,FINTIM,DELT,DTMIN,DTMAX,TPR,TPL
3210 GOTO 21
3215 30 PRINT 300,TITLE
3220 PRINT 120
3225 GOTO 22
3230 20 IF (ABS(TIM-JPR*TPR).GT. DELT*0.3) GOTO 90
3235 JPR=JPR+1
3240 PRINT 170, TIME, JT
3245 21 PRINT 180, PH, CHNA, WHPU, WHCT, RR1
3250 PRINT 190
3255 PRINT 200, (I,LG(I),DC1(I),DC2(I),DC3(I),DC4(I),S1(I),S2(I),S3(I),S
3260 C4(I),C1(I), C2(I),C3(I),C4(I),I=1,50)
3265 25 PRINT 300,TITLE
3270 IF (IPZ.EQ.3) GOTO 99
3275 PRINT 230, (ICT(I),I=1,8)
3280 JTP=0
3285 JTI=0
3290 90 JTI=JTI+1
3295 IF (JTI.LT.JCT) GOTO 99
3300 JTI=0
3305 JTP=JTP+1
3310 DO 91 I=1,8
3315 91 CHX(I)=(0.5*C1(ICT(I))+C4(ICT(I)))*2.0166/(453.6*1E-6)
3320 PRINT 220,JT,TIME,PH,QX,QXT,QHT,ALFA,(CDET(I),I=1,4),(CHX(I),I=2,8
3325 C )
3330 IF (JTP.GT.50) GOTO 25
3335 99 RETURN
3340 100 FORMAT(' *** INITIAL CONDITIONS ***'//)
3345 110 FORMAT(' TIME =',F10.2,' JT =',I10,' FINTIM =',F10.2,
3350 C ' DELT =',F10.4,' DTMIN =',F10.5,' DTMAX =',F10.4/
3355 C ' TPR =',F10.2,' TPL =',F10.2)
3360 120 FORMAT(' *** SIMULATION TERMINATED ***'//)
3365 130 FORMAT(' SEGM TYPE',7X,'SEGMENT PARAMETERS'/
3370 C 10X,' LENGHT CROSS=AREA MASS FLOW LEAK(MOL/SEC'//)
3375 140 FORMAT(I3,2H *,I3,2X,1P5E11.3)
3380 190 FORMAT(1H0,' SEGM TYPE',7X,'SEGMENT DERIVATIVES MOL-SEC-LBS',18X,
3385 C 'SOURCE IN (MOL/SEC)',19X,'CONCENTRATION IN (MOL/LIB)'//
3390 C 10X,' DC1 DC2 DC3 DC4 S1=NAH S2=NAOH
3395 C S3=NA2O S4=H2 C1=NAH C2=NAOH C3=NA2O C4=H2'//)
3400 200 FORMAT(I3,2H *,I3,2X,1P12E10.3)
3405 170 FORMAT(1H1,' SOURCES AND CONCENTRATIONS FOR TIME=',F7.2,' SEC',

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3410      C ' AT ',15,'-TH TIME STEP')
3415      180 FORMAT(' HYDROGEN PARTIAL PRESSURE IN COVER'
3420      C ', ' GAS PH=' ,F10.3, ' MM-HG',10X,'SIEVERTS EQUILIBRIUM H2 IN NA CHN
3425      CA=' ,E12.4, ' (MDL/LB)'/ ' H2 LEAKING FROM THE PUMP TO '
3430      C ', 'COVER WHPU= ' ,E12.4, ' MOLS',11X,'H2 TO GAS PLENUM IN',
3435      C ' CCTL VESEL WHCT=' ,E11.4, ' MOL'/ ' HYDRID DISSOCIATION RATE RR1='
3440      C ',11X,E12.4, ' SEC-1')
3445      210 FORMAT (10E12.4)
3450      220 FORMAT(1X,15,F6.1,F7.4,15F7.3)
3455      230 FORMAT(' STEP TIME PH-(MM) H2O-LK TOT LK TOT H2 ALFA DTCTR1 DTC
3460      CTR2 DTCTR3 DTCTR4 TOTAL HYDROGEN CONCENTRATION IN (PPM) AT NODE #
3465      C ': ',/42X,12,33X,6(12,5X),12)
3470      300 FORMAT(1H1,20(' '),2X,18A4,2X,20(' '))
3475      END
3480
3485 C-----C
3490 C C
3495 C SUBROUTINE SPLOT. C
3500 C IN THIS ROUTINE DATA WILL BE STORED IN FILE 20 EVERY IPL C
3505 C PARAMETER IIP = C
3510 C 1 , INITIAL ENTRY C
3515 C 2 , TIME STEP ENTRY, VALUES STORED C
3520 C 3 , FINAL ENTRY, VALUES RETREIVED AND C
3525 C PRINT-PLOTTED C
3530 C C
3535 C-----C
3540
3545 SUBROUTINE SPLOT(IIP)
3550 C**** THIS SUBROUTINE WILL STORE DATA OF SPECIFIED CONCENTRATION POINTS
3555 C**** AT PREDETERMINED SEGMENTS TO BE PLOTTED LATER ON THE TEXTRONIC
3560 C**** TERMINAL. DATA ARE WRITEN INTO CCTX.DATA=FT20.F001
3565 COMMON /BLK/ L,A,M,C1,C2,C3,C4,LG,WS,WCT,WT1,WT2,WT3,WT4,WEX,TEMP,
3570 C FINTIM,RUNA,DTMIN,DTMAX,S1,S2,S3,S4,JT,KS,TPR,IQ,ICT,W,JCT,
3575 C WR,WA,WX,WB,WC,WD,WE,G,TQ,TX,QS,PDIS,PH,PA,K1,K2,K3,K4,R1,R2,R3,
3580 C WHCT,WHPU,TPLEN,VPLEN,IC,TPL,CHNA,RR1,QX,QXT,QHT,C1SAT,BETA,
3585 C ALFA,TMM,NPCT,NGRAF,NVECT,NAME,IPI,NUDET,NODE,NTYPE,
3590 C TLAG,CDET,TDLE,C3SAT,PDEL,FIGTTL,PTDL,KH
3595 COMMON /LUG/ TITLE,PRT1,PRT2,PRT3,PRT4,PRT5
3600 COMMON /DUB/ TIME,DELT,DC1,DC2,DC3,DC4,ABSC
3605 REAL*4 L(50),A(50),M(50),C1(50),C2(50),C3(50),C4(50),W(50)
3610 REAL*4 S1(50),S2(50),S3(50),S4(50),Q(8),TQ(8),TX(8),QS(50)
3615 REAL*4 K1,K2,K3,K4,KS,TITLE(18),TLAG(7),CDET(7),TDLE(7)
3620 REAL*8 DC1(50),DC2(50),DC3(50),DC4(50),TIME,DELT,ABSC(4,10)
3625 LOGICAL PRT1,PRT2,PRT3,PRT4,PRT5
3630 DIMENSION LG(50),IQ(8),IC(8),ICT(8),NGRAF(10),NVECT(10,5),
3635 C NAME(10,15),IPI(50),NODE(7),NTYPE(7),FIGTTL(15,10)
3640 DIMENSION CCC(10),VMX(55),VECT(55),LINE(121),IL(5),ILX(5),
3645 C DYD(6),IP(5),YZ(4),YW(4),VEPL(250,5),VTIM(250)
3650 LOGICAL L1
3655 DATA JPL/0/,VMX/55*0./,YZ/0.15,0.2,0.5,1.0/,YW/3.,4.,5.,5./
3660 DATA IPO/' ',ICR/'I',IP/'.', '*','+',',',' '#/,IDLR/'S'/
3665 TIM=TIME
3670 GOTO (10,20,30), IIP

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3675      10 REWIND 20
3680      20 IF (ABS(TIM-JPL*TPL).GT,DELT*0.3) GOTO 99
3685      JPL=JPL+1
3690      21 DO 5 I=1,8
3695          5 CCC(I)=(0.5*C1(IC(I))+C4(IC(I)))*2.0166E+6/453.6
3700      WHPT=WHPU+WHCT
3705      EXSC=CHNA/(0.5*C1(27)+C4(27))
3710      VECT(1)=TIM
3715      VECT(2)=ALFA
3720      VECT(3)=QX
3725      VECT(4)=QXT
3730      VECT(5)=WHPT
3735      VECT(6)=EXSC
3740      VECT(7)=PH
3745      VECT(8)=QHT
3750      DO 11 I=1,NUDET
3755      11 VECT(8+I)=CDET(I)
3760      I=0
3765      DO 12 I1=16,51,5
3770      I=I+1
3775      VECT(I1)=C1(IC(I))
3780      VECT(I1+1)=C2(IC(I))
3785      VECT(I1+2)=C3(IC(I))
3790      VECT(I1+3)=C4(IC(I))
3795      VECT(I1+4)=CCC(I)
3800      12 CONTINUE
3805      WRITE (20) VECT
3810      DO 14 I=1,55
3815      14 IF (VECT(I).GT,VMX(I)) VMX(I)=VECT(I)
3820      GOTO 99
3825      30 PRINT 100,JPL
3830      DO 26 N=1,NUDET
3835      NN=8+N
3840      26 PRINT 170,NN,N,NTYPE(N),NODE(N)
3845      I=0
3850      DO 25 JPJ=16,51,5
3855      JPM=JPJ+4
3860      I=I+1
3865      PRINT 110,(J1,IC(I),J1=JPJ,JPM)
3870      25 CONTINUE
3875      PRINT 120, (I,VMX(I),I=1,55)
3880      C
3885      C**** THIS SECTION PREPARES PRINTPLOT
3890      DO 70 NP=1,NPICT
3895      NG=NGRAF(NP)
3900      C**** FIND MAXIMUM VALUE IN PRESENT PICTURE
3905      YS=0.
3910      DO 60 N=1,NG
3915      ILX(I)=0
3920      N1=NVECT(NP,N)
3925      IF (VMX(N1).GT,YS) YS=VMX(N1)
3930      60 CONTINUE
3935      C**** SELECT SCALE FOR GRAPHIC PICTURE

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3940      DO 61 I=1,11
3945      YM=10.**(I-6)
3950      DO 63 II=1,4
3955      YSC=YZ(II)*YM
3960      DYS=YSC/YW(II)
3965      IF(YS.LT.YSC)GOTO 62
3970      63 CONTINUE
3975      61 CONTINUE
3980      62 IDY=DYS/YSC*120.+0.001
3985      PRINT 130,TITLE
3990      PRINT 180,(FIGTTL(I,NP),I=1,15)
3995      PRINT 140,NP,NG
4000      DO 64 N=1,NG
4005      N1=NVECT(NP,N)
4010      PRINT 150,N,N1,IP(N),VMX(N1),(NAME(NP,3*(N-1)+J),J=1,3)
4015      64 CONTINUE
4020      PRINT 220,(ABSC(I,NP),I=1,4)
4025 C**** PRINT SCALES
4030      IS=0
4035      DO 65 I=1,121,IDY
4040      DYD(IS+1)=DYS*IS
4045      IS=IS+1
4050      65 CONTINUE
4055      LAB=IDY/10.-1
4060      GOTO (66,67,68), LAB
4065      66 PRINT 166,(DYD(I),I=1,IS)
4070      GOTO 69
4075      67 PRINT 167,(DYD(I),I=1,IS)
4080      GOTO 69
4085      68 PRINT 168,(DYD(I),I=1,IS)
4090      69 REWIND 20
4095 C**** SET PROPER SIGNAL CHARACTERS INTO LINE
4100      PRINT 210
4105      DO 50 J=1,JPL
4110      READ (20) VECT
4115      VTIM(J)=VECT(1)
4120      DO 52 N=1,NG
4125      N1=NVECT(NP,N)
4130      VEPL(J,N)=VECT(N1)
4135      IL(N)=VECT(N1)/YSC*120
4140      IF(IL(N).LE.0) IL(N)=1
4145      52 CONTINUE
4150      DO 54 I=2,120
4155      54 LINE(I)=IP0
4160      DO 56 I=1,121,IDY
4165      56 LINE(I)=ICR
4170      IF(VECT(3).EQ.0.0) GOTO 53
4175      DO 73 I=2,8
4180      73 LINE(I)=IDLr
4185      53 DO 51 N=1,NG
4190      IF(NG.NE.1) GOTO 59
4195      IF(IL(N).EQ.ILX(N)) GOTO 59
4200      IF(IL(N).LT.ILX(N)) GOTO 57

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4205      I1=ILX(N)+1
4210      I2=IL(N)
4215      GOTO 58
4220      57 I1=IL(N)
4225      I2=ILX(N)-1
4230      58 DO 55 I=I1,I2
4235      55 LINE(I)=IP(N)
4240      59 LINE(IL(N))=IP(N)
4245      ILX(N)=IL(N)
4250      51 CONTINUE
4255      PRINT 200,VECT(1),LINE
4260      50 CONTINUE
4265      PRINT 211
4270      IF(PRT5) CALL PLOTTER(JPL,NP,NG,VEPL,VTIM,YS,TIM,YSC,DYS,FIGTTL,
4275      C  ABSC,NAME,NPICT)
4280      70 CONTINUE
4285      99 RETURN
4290      100 FURMAT (1H0,3(/),1H ,20('*'),16,' RECORDS ARE WRITEN FOR PLOTTING
4295      C  ',20('*'))//10X,'#01 TIME (SEC)'/10X,'#02 ALFA'/10X,
4300      C  '#03 LEAK H2O (MOL/SEC)'/10X,'#04 TOTAL H2O LEAK (MOL)'/
4305      C  10X,'#05 H2 FLOW TO PLENUM (MOL/SEC)'/10X,
4310      C  '#06 EXCESS H2 IN COVER GAS OVER NODE 27'/10X,
4315      C  '#07 H2 PARTIAL PRESSURE IN COVER GAS (MM-HG)'/10X,
4320      C  '#08 TOTAL HYDROGEN IN CCTL SYSTEM (MOL)')
4325      110 FORMAT(' CONC (MOL/LB)  #',I2,' C1(',I2,')-NAH  #',I2,
4330      C  ' C2(',I2,')-NAOH  #',I2,' C3(',I2,')-NA2O  #',I2,' C4('
4335      C  ',I2,')-H2  #',I2,' DETECTABLE H IN NODE ',I2,' (PPM)')
4340      120 FORMAT('THE APPROPRIATE MAXIMUM VALUES OF THE VARIABLES ARE'/
4345      C  11(11X,5(4X,'#',I2,1PE12.3)/))
4350      130 FORMAT(1H1,20('*'),18A4,20('*'))
4355      140 FORMAT(' PICTURE #',I2,' HAS ',I2,' GRAPHS')
4360      150 FORMAT(' GRAPH #',I2,' IS VECT(',I2,'), SYMBOL IS ',A1,' MAX=',
4365      C  E11.4,3X,3A4)
4370      166 FORMAT(1X,F10.1,5(14X,1PE10.3))
4375      167 FORMAT(1X,F10.1,4(20X,1PE10.3))
4380      168 FORMAT(1X,F10.1,3(30X,1PE10.3))
4385      170 FORMAT(10X,'#',I2,' RESPONSE OF DETECTOR ',I2,' IN (PPM). TYPE'
4390      C  ',IS ',I1,' CONNECTED TO NODE ',I2)
4395      180 FORMAT(40X,15A4)
4400      200 FORMAT(1X,F7.2,3X,121A1)
4405      210 FORMAT(4X,'TIME',3X,121(' '))
4410      211 FORMAT(11X,121(' '))
4415      220 FORMAT(1H0,40X,4A8)
4420      END
4425
4430
4435 C -----C
4440 C SUBROUTINE PIPE. C
4445 C IN THIS ROUTINE PIPE FUNCTION ARE STORED. PIPE LAG FUNCTIONS C
4450 C ARE THEN CALCULATED BY LINEAR INTERPOLATION BETWEEN THE TWO C
4455 C VALUES CLOSEST TO TIME TAU. C
4460 C THE PARAMETERS ARE : C
4465 C TIME = CURRENT SIMULATION TIME C

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4470 C          DELT = TIME STEP INCREMENT
4475 C          TAU = TIME LAG FOR WHICH PIPE FUNCTION IS REQUIRED
4480 C          IP  PIPE FUNCTION NUMBER (1-9)
4485 C          FX1,FX2,FX3,FX4 = CALCULATED PIPE FUNCTIONS FOR TIME-TAU
4490 C                               OR UPDATE VALUES IF TAU=0.0
4495 C
4500 C-----
4505
4510          SUBROUTINE PIPE(TIME,DELT,TAU,IP,FX1,FX2,FX3,FX4)
4515          COMMON /LUG/ TITLE,PRT1,PRT2,PRT3,PRT4
4520          LOGICAL PRT1,PRT2,PRT3,PRT4,PRT5
4525          DIMENSION F(10,4,100),CONCN(4),T(100),TITLE(18)
4530          LOGICAL L1,L2
4535          DATA L1,L2/2*.FALSE./,CONCN/'NAH ','NAUH','NA2D','H2 '/
4540          IF(L1) GOTO 2
4545          L1=.TRUE.
4550          DO 4 I=1,100
4555          T(I)=(I-100)*DELT*10.0
4560          DO 3 IP=1,9
4565          F(IP,1,I)=FX1
4570          F(IP,2,I)=FX2
4575          F(IP,3,I)=FX3
4580          F(IP,4,I)=FX4
4585          3 CONTINUE
4590          4 CONTINUE
4595          GOTO 99
4600          2 IF(L2) GOTO 5
4605          L2=.TRUE.
4610          DO 1 I=1,100
4615          F(10,1,I)=FX1
4620          F(10,2,I)=FX2
4625          F(10,3,I)=FX3
4630          F(10,4,I)=FX4
4635          1 CONTINUE
4640          GOTO 91
4645 C**** UPDATE THE PIPE FUNCTIONS FOR PRESENT TIME
4650          5 IF(TAU.NE.0.0) GOTO 10
4655          IF(TIME.EQ.T(100)) GOTO 22
4660          DO 8 I=1,99
4665          T(I)=T(I+1)
4670          T(100)=TIME
4675          22 DO 20 K=1,4
4680          DO 20 I=1,99
4685          20 F(IP,K,I)=F(IP,K,I+1)
4690          F(IP,1,100)=FX1
4695          F(IP,2,100)=FX2
4700          F(IP,3,100)=FX3
4705          F(IP,4,100)=FX4
4710          GOTO 99
4715 C**** SEARCH FOR PIPE OUTPUT CONCENTRATION AT PRESENT TIME (TIME-TAU)
4720          10 J=0
4725          DEL=TIME-T(100)
4730          IF(TAU.GT.DEL) GOTO 15

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4735      J=100
4740      TDEL=DEL-TAU
4745      IF (ABS(TDEL).LT.0.001) GOTO 13
4750      DTD=(T(100)-T(99)+TDEL)/(T(100)-T(99))
4755      DP=DTD
4760      DM=1.-DTD
4765      GOTO 12
4770 15 TDEL=TIME-TAU
4775      IF (TDEL.LT.T(1)) GOTO 90
4780 9   J=J+1
4785      IF (ABS(T(J)-TDEL).LE.0.001) GOTO 13
4790      IF (T(J).GE.TDEL) GOTO 11
4795      GOTO 9
4800 11 DT=T(J)-T(J-1)
4805      DTD=T(J)-TDEL
4810      DP=DTD/DT
4815      DM=1.-DP
4820 12 FX1=F(IP,1,J-1)*DM+F(IP,1,J)*DP
4825      IF (IP.EQ.10) GOTO 99
4830      FX2=F(IP,2,J-1)*DM+F(IP,2,J)*DP
4835      FX3=F(IP,3,J-1)*DM+F(IP,3,J)*DP
4840      FX4=F(IP,4,J-1)*DM+F(IP,4,J)*DP
4845      GOTO 99
4850 13 FX1=F(IP,1,J)
4855      FX2=F(IP,2,J)
4860      FX3=F(IP,3,J)
4865      FX4=F(IP,4,J)
4870      GOTO 99
4875 C*** ERROR OUTPUT
4880 91 IF (PRT1) GOTO 92
4885      GOTO 99
4890 90 PRINT 100,TIME,TAU,IP,T(1)
4895 92 PRINT 110,((CUNCN(K),J,T(J),(F(IP,K,J),IP=1,10),J=1,100),K=1,4)
4900 99 RETURN
4905 100 FORMAT(1H1,1H ,125(' '),'/' ERROR AT TIME=',F10.4/
4910      C ' PIPE DELAY IS TAU=',F10.4,'PIPE IS SEGMENT NUMBER ',I3/
4915      C ' FIRST VALUE IN PIPE SEGMENT IS GIVEN AT TIME=',F10.4/1H ,132(' *
4920      C '))
4925 110 FORMAT ('1'/' PIPE FUNCTIONS'/' MAT INDX   TIME      SECT=1',10X,'3
4930      C',10X,'23',10X,'27',9X,'29',9X,'6',9X,'25',9X,'NU',9X,'NU',6X,'RR1
4935      C,PH,CHNA'/(1X,A4,I5,0PF12.5,1P10E11.3))
4940 200 FORMAT (1X,3E12.4,2I6,4E12.4)
4945      END
4950
4955 C-----C
4960 C
4965 C      SUBROUTINE DETECT.
4970 C      IN THIS ROUTINE THE DIRECTOR RESPONSE IS COMPUTED. THREE
4975 C      TYPES ARE ACCOUNTED FOR: HYDROGEN IN NA, HYDROGEN IN COVER
4980 C      GAS, AND OXYGEN. THE RESPONSE IS GIVEN IN PPM WEIGHT FOR THE
4985 C      SOLUTION AND PPM-VOLUME FOR THE COVER GAS.
4990 C
4995 C-----C

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5000
5005      SUBROUTINE DETECT
5010 C
5015      COMMON /BLK/ L,A,M,C1,C2,C3,C4,LG,WS,WCT,WT1,WT2,WT3,WT4,WEX,TEMP,
5020      C FNTIM,RUNA,DTMIN,DTMAX,S1,S2,S3,S4,JT,KS,TPR,IQ,ICT,W,JCT,
5025      C WR,WA,WX,WB,WC,WD,WE,Q,TQ,TX,QS,POIS,PH,PA,K1,K2,K3,K4,R1,R2,R3,
5030      C WHCT,WHPU,TLEN,VLEN,IC,TPL,CHNA,RR1,QX,QXT,QHT,C1SAT,BETA,
5035      C ALFA,TMM,NPICT,NGRAF,NVECT,NAME,IPI,NUDET,NODE,NTYPE,
5040      C TLAG,CDET,TDLE,C3SAT,PDEL,FIGTTL,PTDL,KH
5045      COMMON /LUG/ TITLE,PRT1,PRT2,PRT3,PRT4,PRT5
5050      COMMON /DUB/ TIME,DELT,DC1,DC2,DC3,DC4,ABSC
5055      REAL*4 L(50),A(50),M(50),C1(50),C2(50),C3(50),C4(50),W(50)
5060      REAL*4 S1(50),S2(50),S3(50),S4(50),Q(8),TQ(8),TX(8),QS(50)
5065      REAL*4 K1,K2,K3,K4,KS,TITLE(18),TLAG(7),CDET(7),TDLE(7)
5070      REAL*8 UC1(50),DC2(50),DC3(50),DC4(50),TIME,DELT,ABSC(4,10)
5075      LOGICAL PRT1,PRT2,PRT3,PRT4,PRT5
5080      DIMENSION LG(50),IQ(8),IC(8),ICT(8),NGRAF(10),NVECT(10,5),
5085      C NAME(10,15),IPI(50),NODE(7),NTYPE(7),FIGTTL(15,10)
5090      TIM=TIME
5095      DEL=DELT
5100      DO 10 N=1,NUDET
5105      LTP=NTYPE(N)
5110      IF(LTP.EQ.3) GOTO 15
5115      N1=NODE(N)
5120      IP=IPI(N1)
5125      TAU=M(N1)/W(N1)+TLAG(N)
5130      IF(TAU.GT.TIME) TAU=TIME
5135      CALL PIPE(TIM,DEL,TAU,IP,FX1,FX2,FX3,FX4)
5140      CALL PIPE(TIM,DEL,TAU,10,X1,X2,X3,X4)
5145      SD1=-(X1+WR1)/2.*FX1
5150      SD2=-R3*FX2
5155      SD3=-SD2
5160      SD4=-(SD1+SD2)*0.5
5165      CD1=(FX1+SD1*TAU)*1.0083E+6/453.6
5170      CD2=(FX2+SD2*TAU)
5175      CD3=(FX3+SD3*TAU)*16.0E+6/453.6
5180      CD4=(FX4+SD4*TAU)*2.0166E+6/453.6
5185      GOTO 19
5190      15 CD4=PH*1.0E+6/(PH+PA)
5195      19 GOTO (20,30,40), LTP
5200 C*** HYDROGEN DETECTOR
5205      20 DPP=(CD1+CD4-CDET(N))/TDLE(N)
5210      CALL INTG1(N,CDET(N),DPP,DELT)
5215      GOTO 10
5220 C*** OXIGEN DETECTOR
5225      30 DPP=(CD3-CDET(N))/TDLE(N)
5230      CALL INTG1(N,CDET(N),DPP,DELT)
5235      GOTO 10
5240 C*** HYDROGEN GAS DETECTOR
5245      40 DPP=(CD4-CDET(N))/TDLE(N)
5250      CALL INTG1(N,CDET(N),DPP,DELT)
5255 C*** OTHER TYPES OF DETECTORS
5260      10 CONTINUE

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5265      99 RETURN
5270      END
5275      SUBROUTINE PLOTTER(J,NP,NN,X,T,YMX,TF,YSC,DYS,FIGTTL,ABSI,NAME,
5280      C NPIC1)
5285 C -----
5290 C
5295 C      SUBROUTINE PLUTER
5300 C      IN THIS ROTINE A FIGURE ON THE CALCOMP PLOTTER IS PREPARED
5305 C      PARAMRTIERS ARE:
5310 C          J - NUMBER OF POINTS IN VECTOR TO BE DRAWN
5315 C          NP - FIGURE NUMBER
5320 C          NN - NUMBER OF CURVES IN FIGURE
5325 C          X - VECTOR INCLUDING THE CURVES
5330 C          T - THE TIME VECTOR
5335 C          YMX - MAXIMUM VALUE OF VECTORS TO BE DRAWN
5340 C          TF - TOTAL/FINAL TIME OF THE PLOT
5345 C          YSC - SCALE OF THE ABSCISAE
5350 C          HEAD - FIGURE HEADING
5355 C          ABSC - ABSCISAE HEADING
5360 C          NAME - NAME OF CURVES - LEGEND
5365 C -----
5370 C
5375      DIMENSION X(250,5),T(250),HEAD(15),NAMS(3),TL(2),TI(250)
5380 C      ,Z(250),NAME(10,15),IPAK(200),FIGTTL(15,10)
5385      REAL*8 ABSI(4,10),ABSC(4)
5390      DATA KP/0/
5395      TF5=TF/5.
5400      TL(1)=TF/25.
5405      TL(2)=TF5-TL(1)
5410      TI=0.
5415      TX=TF
5420      J1=1
5425      J2=J
5426 C
5427 C**** INSERT ALL TITLES IN PROPER VECTORS FOR PLOTTER DRAWING
5430      DO 1 I=1,15
5435      1 HEAD(I)=FIGTTL(I,NP)
5440      DO 2 I=1,4
5445      2 ABSC(I)=ABSI(I,NP)
5450      IF(NP.GT.1) GOTO 12
5455      CALL STRTPL
5460      12 KP=KP+1
5465      CALL BGNPL(KP)
5470      DO 17 N=1,NN
5475      DO 16 K1=1,3
5480      N3=(N-1)*3+K1
5485      16 NAMS(K1)=NAME(NP,N3)
5490      CALL LINES(NAMS,IPAK,N)
5495      17 CONTINUE
5500      CALL TITLE(1H , -1, 'TIME(SEC)',9,ABSC,32,8.,6.)
5505      CALL HEADIN(HEAD,100,3,1)
5510      CALL GRAF(TI,TF5,TX,0.0,DYS,YSC)
5515      UY=5.3-0.3*NN

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5520      CALL BLNK1(5.0,7.8,UY,5.8,2)
5525      CALL GRID(1,1)
5530      CALL FRAME
5535      DO 40 N=1,NN
5540      DO 10 I=1,J
5545      Z(I)=X(I,N)
5550      10 CONTINUE
5555      I=0
5560      DO 42 J3=J1,J2
5565      I=I+1
5570      Z(I)=Z(J3)
5575      T1(I)=T(J3)
5580      42 CONTINUE
5585      NM=2*N+20
5590      CALL CURVE(T1,Z,J,NM)
5595      40 CONTINUE
5600      CALL RESET('BLNK1')
5605      UY2=UY+0.2
5610      CALL LEGEND(IPAK,NN,5.2,UY2)
5615      CALL ENDPL(KP)
5620      IF(KP.LT.NP1CT) GOTO 99
5625      CALL DONEPL
5630      99 RETURN
5635      END
5640 C-----
5645 C
5650 C      BLOCK DATA
5655 C      IN THIS ROUTINE DEFAULT AND OTHER INITIAL DATA ARE PLACED
5660 C
5665 C-----
5670 C
5675      BLOCK DATA
5680      COMMON /BLK/ L,A,M,C1,C2,C3,C4,LG,WS,WCT,WT1,WT2,WT3,WT4,WEX,TEMP
5685      C FINTIM,RONA,DTMIN,DTMAX,S1,S2,S3,S4,JT,KS,IPR,IQ,ICT,W,JCT,
5690      C WR,WA,WX,WB,WC,WD,WE,Q,TQ,TX,QS,PDIS,PH,PA,K1,K2,K3,K4,R1,R2,R3,
5695      C WHC1,WHPU,TLEN,VLEN,IC,TPL,CHNA,RR1,QX,QXT,QHT,C1SAT,BETA,
5700      C ALFA,TMM,NP1CT,NGRAF,NVECT,NAME,IPI,NUDET,NODE,NTYPE,
5705      C TLAG,CDET,TDLE,C3SAT,PDEL,FIGTTL,PTDL,KH
5710      COMMON /LOG/ TITLE,PRT1,PRT2,PRT3,PRT4,PRT5
5715      COMMON /DUB/ TIME,DELT,DC1,DC2,DC3,DC4,ABSC
5720      REAL*4 L(50),A(50),M(50),C1(50),C2(50),C3(50),C4(50),W(50)
5725      REAL*4 S1(50),S2(50),S3(50),S4(50),Q(8),TQ(8),TX(8),QS(50)
5730      REAL*4 K1,K2,K3,K4,KS,TITLE(18),TLAG(7),CDET(7),TDLE(7)
5735      REAL*8 DC1(50),DC2(50),DC3(50),DC4(50),TIME,DELT,ABSC(4,10)
5740      LOGICAL PRT1,PRT2,PRT3,PRT4,PRT5
5745      DIMENSION LG(50),IQ(8),IC(8),ICT(8),NGRAF(10),NVECT(10,5),
5750      C NAME(10,15),IPI(50),NODE(7),NTYPE(7),FIGTTL(15,10)
5755 C**      DEFAULT VALUES
5760      DATA BETA/0.001/,
5765      C      C1SAT/1.418E-6/,
5770      C      CDET/7*0.0/,
5775      C      DTMAX/1.0/,
5780      C      DTMIN/0.005/,

```

CCTL,FORT

```
5785 C      JT/0/
5790 DATA PDEL/0.01/,
5795 C      PRT1,PRT2,PRT3,PRT4,PRT5/5*.FALSE./,
5800 C      Q/8*0.0/,
5805 C      TIME/0.0/,
5810 C      TG/8*10.0/,
5815 C      TX/8*80.0/,
5820 C      WT1,WT2,WT3,WT4/4*0.0/
5825 END
```

APPENDIX D

The Input Data; How to Run CCTL-DYSP1. Title

The first line is a title of 72 characters and will be printed at the top of each output page.

2. INLIST

The data in this section are inserted in a free NAMELIST format. All the data are single variables or vectors, and should be placed between

Δ &INLIST Δ * as a first card, and

Δ &END as the last card.

All the vectors can be input as whole vectors

$x = a_1, a_2, \dots, a_{50},$

or single members; e.g.,

$x(5) = a_5; x(7) = a_7.$

In the first case, all elements of the vectors have to be supplied. (The variables can be input in any order.)

$L(50) =$ CCTL segment length, in feet;

$LG(50) =$ a logic variable, which determines the type of segment

= 0 the segment is excluded from the simulation

= 1 plenum mixing segment

= 2 pipe segment

= 3 plenum mixing with cover gas

= 4 multiple-entry mixing plenum

= 5 multiple-entry mixing plenum with cover gas;

$A(50) =$ segment cross section area, in ft^2 ;

$C1(50) =$ NaH concentration, in ppm;

$C2(50) =$ NaOH concentration, in ppm;

$C3(50) =$ Na_2O concentration, in ppm;

$C4(50) =$ hydrogen concentration, in ppm.

* Δ indicates a space.

Only the first value for each of C1(1), C2(1), and C3(1), and C4(1) has to be input to calculate the initial distribution in the system.

- Q(8) = leak at the Ith injection point, in lb/sec;
- QT(100) = normalized time-dependent leak function;
- TQ(8) = time, in seconds, when the leak at node I starts;
- TQT(100) = time table at which normalized leak-function values are given;
- TX(8) = time (in seconds) when the leak at node I is terminated;
- IQ(8) = CCTL node number at which leak might occur, i.e., nodes at which nozzles were installed;
- IC(8) = node numbers for which detailed concentration information will be stored in CCTX.DATA file for future plotting; the nodal information stored includes C1, C2, C3, C4, and detectable hydrogen concentrations, in ppm;
- ICT(8) = nodes for which hydrogen concentration will be printed every JCT time steps; for ICT(1), however, ALFA will be printed.

3. PARM

The data in this section are system parameters and are inserted in a free NAMELIST format. These are scalar variables. If they will not be included in the input stream, the default value (usually 0) will be assumed by the program. The parameters should be placed between

Δ &PARM Δ as the first card, and

Δ &END as the last card, and should be separated by commas.

TEMP = sodium temperature, in °F;

WS = total sodium flow, in gal/min;

WCT = flow through the cold trap, in gal/min;

WT1 = flow toward the detectors from node 6;

WT2 = to be determined;

WT3 = flow toward the detectors from node 23, in gal/min;

WT4 = flow toward the detectors from node 25, in gal/min;

WEX = sodium leak between nodes 3 and 22, in gal/min;

PDEL = maximum permitted change in node 23 for pipe update;

PTDL = maximum time interval at which pipe is updated;

PRT1 = (Logical) if TRUE, initial pipe-function distribution will be printed;
 PRT5 = (Logical) if TRUE, time-dependent results arranged for print-plot also will be plotted on the CALCOMP plotter;
 TCLT = Cold-trap temperature;
 PH = Hydrogen partial pressure in cover gas, in mm Hg;
 PA = Argon partial pressure in cover gas, in mm Hg;
 FINTIM = simulation time, in seconds;
 DELT = single integration time step, in seconds;
 DTMIN = minimum permitted time step, in seconds;
 DTMAX = maximum permitted time step, in seconds;
 VPLEN = total gas plenum volume, in ft³;
 TPR = printing time interval for complete concentration map, in seconds;
 TPL = time intervals at which an entry for plotting is calculated, in seconds;
 JCT = number of time steps between two consecutive printings of detectable hydrogen concentration and meter readings (a single line is printed every JCT time steps);
 K1 = fraction of water leak to $\text{Na} + \text{H}_2\text{O} \rightarrow \text{NaOH} + \frac{1}{2}\text{H}_2$, reaction;
 K2 = fraction of water leak to $2\text{Na} + \text{H}_2\text{O} \rightarrow \text{NaOH} + \text{NaH}$, reaction;
 K3 = fraction of water leak to $4\text{Na} + \text{H}_2\text{O} \rightarrow 2\text{NaH} + \text{H}_2\text{O}$, reaction;
 K4 = fraction of water leak to $2\text{Na} + \text{H}_2\text{O} \rightarrow \text{Na}_2\text{O} + \text{H}_2$, reaction;
 R1 = rate of hydrogen disengagement from liquid sodium to cover gas, in sec⁻¹;
 BETA = cold-trap static efficiency;
 R3 = rate of NaOH dissociation, in sec⁻¹.

4. DTCTR

This section contains a list of parameters describing the detectors monitoring CCTL. Parameters are inserted in free NAMELIST format and should be placed between

Δ DTCTR Δ as the first card, and

Δ END as the last card, and should be separated by commas.

NUDET = number of detectors in present simulation (maximum is 7);
 NODE(7) = the node number to which detector is attached;
 NTYPE(7) = type of detector
 1 = hydrogen detector in sodium
 2 = oxygen detector in sodium
 3 = hydrogen-gas detector in cover gas;
 TDLE(7) = diffusion time constant for the nickel membrane, in seconds;
 TLAG(7) = time lag between detector sample line inlet and detector, in seconds.

5. Print-Plot Data

These data will direct the printing of time-dependent plots. If TPRS is true, then graphic output on a CALCOMP plotter also will be generated. The data must be input in the formats described below.

CARD 1 = The first card can be any comment of up to 80 characters.
 CARD 2 = NPICT;FORMAT(I2), number of pictures to be printed.
 CARD 3 = NGRAF(10);FORMAT(10(I2, 1X)), NPICT numbers each giving the number of curves to be drawn in a picture.
 CARD 4-I = NVECT(10);FORMAT(10(I2, 1X))

These numbers from 2 to 55 give the position of the variables to be drawn in the 55-place vector VECT as written in the CCTX.DATA file.

#1: time (sec)
 #2: ALFA defined by $(C1(I) + C2(I))/\text{average total hydrogen concentration in the loop}$
 #3: water leak (mol/sec)
 #4: total water leak (mol)
 #5: hydrogen flow to the cover gas (mol/sec)
 #6: excess hydrogen in cover gas over node 27 (mm Hg)
 #7: hydrogen partial pressure in cover-gas plenum (mm Hg)
 #8: total hydrogen in the CCTL system (mol)
 #9-15: detector readings (ppm)
 #16: NaH concentration in the IC(1)th node (mol/lb)
 #17: NaOH concentration in the IC(1)th node (mol/lb)

#18: Na₂O concentration in the IC(1)th node (mol/lb)
 #19: hydrogen concentration in the IC(1)th node (mol/lb)
 #20: detectable hydrogen concentration in the IC(1)th node (ppm)
 #21-25: same as #16-20, but for IC(2)th node
 #26-30: same as #16-20, but for IC(3)th node
 #31-35: same as #16-20, but for IC(4)th node
 #36-40: same as #16-20, but for IC(5)th node
 #41-45: same as #16-20, but for IC(6)th node
 #46-50: same as #16-20, but for IC(7)th node
 #51-55: same as #16-20, but for IC(8)th node

CARD 5-I = NAME(10):FORMAT(5(3A4, 1X)): names to be assigned to each curve; must be terminated by \$

CARD 6-I = ABSC(10):FORMAT(4A8): 32 alphameric characters to be printed along the abscissa of the picture

CARD 7-I = FIGTTL(10):FORMAT(15A4): title to be given to the Ith figure can be up to 60 characters and must be terminated by \$. Card sequences 4-5-6 are repeated NPICT times.

CARD 8 (A4) = 9999: this is the last card indicating the end of the data input.

A sample input data set is shown below.

6. Sample Input Data Set

```
RUN # 24: CCTLP LEAK DETECTION SIMULATION.(.015LB/SEC AT INJ#4, DUR=5SEC)
&INLST L=1., 40.9, 1., 10., 1., 1., .2775, .4171,
.4021, .4588, .7788, .8546, .7788, .7221, .7221,
.7788, .8546, .7788, .4588, .4021, .4171, .3889,
1., 2.89, 1.0, 2.083, 7.5, 19.0, .8,
31.,
10*1.0,
28.0, 1.0, 16.0, 16., 0.0, 0.0, 18.585,
36.87, 42.67, 42.26,
A= 1.069, .09893, .3395, .09893, .2127, 1.49,
16*0.324,
.2127, .09893, 4.03, 6.335, 6.445, .15255, .15255,
.15255,
10*0.0
0.00248, 3.276, 0.00248, .1796, .0, .0,
4*0.00248,
LG= 3, 2, 1, 2, 1, 16*1,4,1, 2, 2*1, 5, 2, 4, 2, 0, 9*0,
2, 1, 2, 0, 0, 0, 2, 2, 2, 2,
```



```

C1(1)=75.E-9,
C2(1)=1.E-9,
C3(1)=35.E-6,
C4(1)=1.E-8,
Q(4)=0.015,
TX(4)=15.0,
TQ(4)=10.0,
IQ=22, 19, 17, 16, 15, 12, 10, 6,
IC=16, 6, 49, 23, 47, 1, 27, 29,
ICT=47, 6, 49, 23, 47, 16, 27, 1,

&END
&PARAM TEMP=900.,WS=800.,WCT=4.,WT1=5.,BETA=0.9,WT3=5.0,WEX=1.,
FINTIM=120.,DELT=0.05,TPR=20.0, TCLT=240.0, PDEL=0.10,
PH=0.1, PA=800.0, K1=0.45, K2=0.2, K3=0.25, K4=0.1, R1=9.625E-6,
R3=7.5E-5, VPLEN=40., TPL=0.5, JCT=10, PRT5=.TRUE.,

&END
&DTCR NUDET=4,
NODE(1)=49, NODE(2)=49, NODE(3)=47, NODE(4)=27,
NTYPE(1)=1, NTYPE(2)=2, NTYPE(3)=1, NTYPE(4)=3,
TLAG(1)=10.0, TLAG(2)=12.0, TLAG(3)=10.0, TLAG(4)=1.0,
TDLE(1)=14.0, TDLE(2)=15.0, TDLE(3)=14.0, TDLE(4)=10.0,

&END
***** DATA FOR PRINT PLOT FOLLOW. LAST CARD MUST BE '9999' *****
04
04,04,05,02
20,35,40,11
AT NODE 16 $,AT NODE 23 $,AT NODE 47 $,AT NODE 27 $
HYDROGEN CONCENTRATION IN (PPM)
HYDROGEN TRANSIENT CONCENTRATION RESPONSE TO .075LB LEAK$
36,37,38,39
NAH AT # 23$,NAOH AT #23$,NA2O AT #23$,H2 AT # 23 $
REACTION PRODUCTS CONC. IN (PPM)
CHANGES IN REACTION PRODUCTS IN RESPONSE TO .075 LB LEAK$
09,11,20,45,50
H-DETECTOR1$,H-DETECTOR3$,INJECTOR J4$,PUMP NODE $,CCTL VESSEL$
HYDROGEN CONCENTRATION IN (PPM)
DETECTOR READINGS RESULTING FROM .075LB LEAK-INJECTOR J4$
10,12
H-DETECTOR2$,0-DETECTOR4$
DETC2 IN (WPPM); DETC4 IN (VPPM)
H-DETECTORS READING IN COVER GAS AND STEAM GENERATOR TUP$
9999
/*

```

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